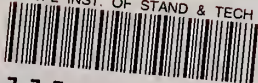


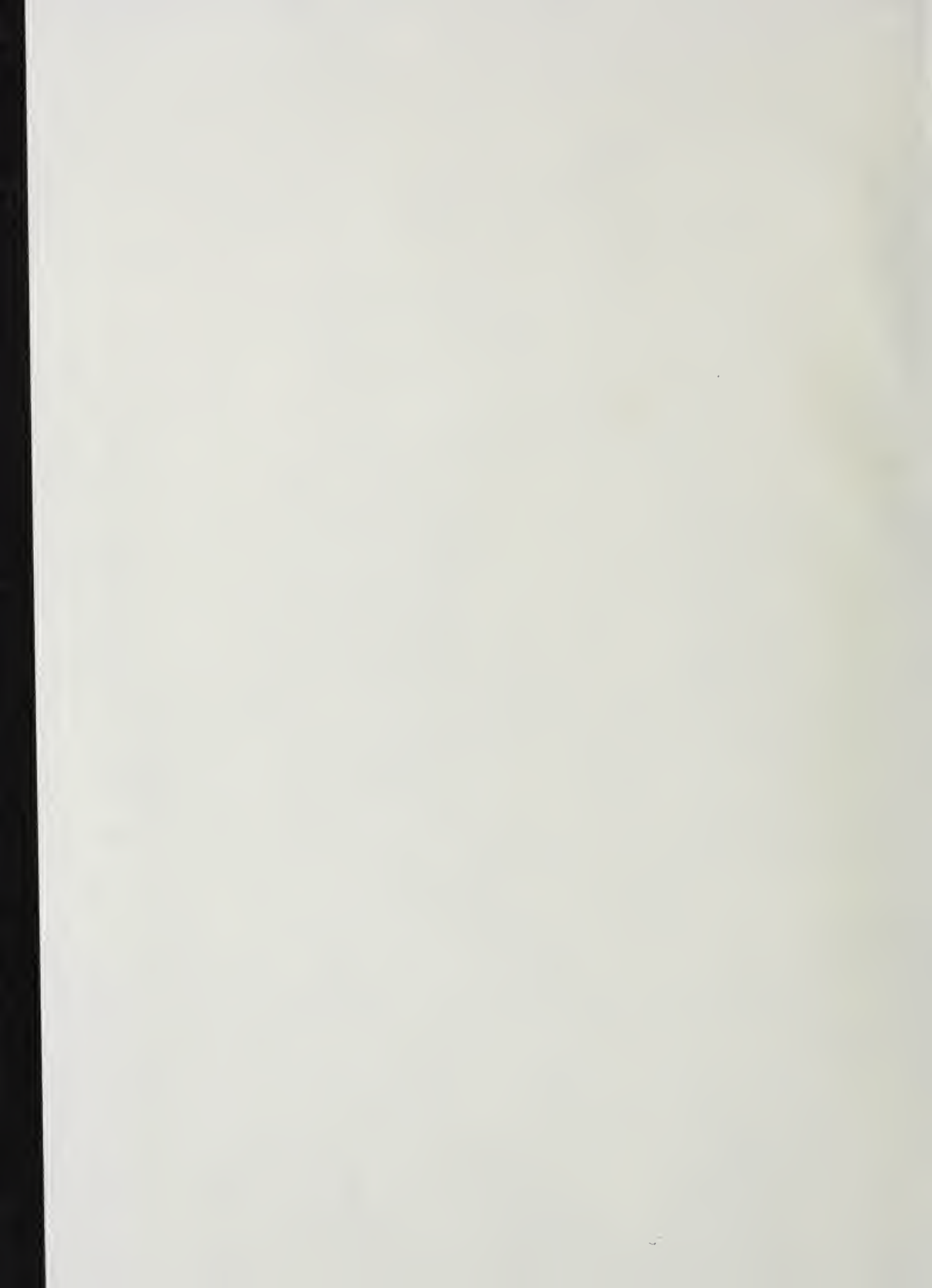
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## Reaction Rate and Photochemical Data for Atmospheric Chemistry - 1977





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# Reaction Rate and Photochemical Data for Atmospheric Chemistry - 1977

*Special publication no. 513*

Edited by

Robert F. Hampson, Jr. and David Garvin

National Measurement Laboratory  
National Bureau of Standards  
Washington, D.C. 20234

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## FOREWORD

The National Standard Reference Data System was established in 1963 for the purpose of promoting the critical evaluation and dissemination of numerical data of the physical sciences. The program is coordinated by the Office of Standard Reference Data of the National Bureau of Standards, but involves the efforts of many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated numerical data. These tables are published in the Journal of Physical and Chemical Reference Data, The NSRDS-NBS Publication Series of the National Bureau of Standards, and through other appropriate channels.

The present report consists of tables of data assembled for use in modelling the chemistry of the stratosphere. It represents contributions from the Chemical Kinetics Information Center, other NSRDS data centers, and a number of individual experts. Support for the preparation of those tables has been provided by the Department of Transportation under the High Altitude Pollution Program, by the National Aeronautics and Space Administration under the Upper Atmosphere Research Program, and by the Office of Standard Reference Data, N.B.S. and the Office of Environmental Measurements, N.B.S.

David R. Lide, Jr.  
Chief, Office of Standard  
Reference Data

## TABLE OF CONTENTS

Abstract	1
1. Introduction	1
2. Guide to the Table	3
3. Reaction Index	9
4. Table. Data for chemical reactions and photochemistry of neutral species	16
5. Reference List	67
<u>Appendices:</u>	
1. Chemical Thermodynamic Properties of Selected Molecular Species	90
2. Conversion Tables	104

R. F. Hampson, D. Garvin, Editors

A table of data for gas phase chemical reactions and photochemistry of neutral species is presented. Specifically, it gives preferred values for reaction rate constants, photoabsorption cross sections, and quantum yields of primary photochemical processes and also cites recent experimental work (to December 1977). It is intended to provide the basic physical chemical data needed as input data for calculations modelling atmospheric chemistry. An auxiliary table of thermochemical data for the pertinent chemical species is given in the appendix.

Key words: Air pollution; atmospheric chemistry; chemical kinetics; data evaluation; gas phase; photoabsorption cross section; photochemistry; quantum yield; rate constant.

## 1. Introduction

This technical note consists of a table of data on the kinetics of chemical reactions and the photochemistry of neutral species. It is designed for use in modelling the chemistry of the stratosphere and, to a more limited extent, the polluted troposphere and also the interpretation of laboratory experiments. The table of rate and photochemical data is supplemented by a table of thermochemical data for the species involved.

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\* This work was supported by the High Altitude Pollution Program of the Federal Aviation Administration, U. S. Department of Transportation, by the Upper Atmospheric Research Program of the National Aeronautics and Space Administration, and by the Office of Standard Reference Data, N.B.S. and the Office of Environmental Measurements, N.B.S.



Earlier versions of this table have been issued as D. Garvin (editor) "Chemical Kinetics Data Survey IV" NBSIR 73-203 (1973); D. Garvin and R. F. Hampson (editors) "Chemical Kinetics Data Survey VII" NBSIR 74-430 (1974); and R. F. Hampson and D. Garvin (editors) "Chemical Kinetic and Photochemical Data for Modelling Atmospheric Chemistry" NBS Technical Note 866 (1975). The table appearing in NBS Technical Note 866 was also published in the U. S. Department of Transportation's Climatic Impact Assessment Program Monograph 1 "The Natural Stratosphere of 1974" E. Reiter, editor (1975). The present table supersedes all earlier versions.

Since the publication of NBS Technical Note 866 in 1975, a major effort in the evaluation of rate and photochemical data was undertaken for the NASA chlorofluoromethane assessment by its Laboratory Measurements Committee of which the present editors were members. The recommendations of this committee covering 104 chemical reactions and 48 photochemical processes are given in NASA Reference Publication 1010 "Chlorofluoromethanes and the Stratosphere" R. D. Hudson, editor, August 1977. These recommendations have been accepted by the editors of this table and are given here as preferred values. These recommendations are indicated either by the entry [ $\dagger$ \*NASA(1977)eval] or by the symbols [ $\dagger$ \*] immediately preceding the author's name in the reference column. The first notation is used to indicate that the committee has synthesized a preferred value from a consideration of all data sets. The latter designation is used when the committee has accepted the results of a particular study or of an existing evaluation.

Recommended values also are given for reactions not considered by the NASA Laboratory Measurements Committee. Some of these are drawn from other modern rate data evaluations, and the sources are indicated in the table. Other recommendations have been prepared for this work.

Rate data evaluation is a small but growing branch of physical chemistry. There are more recommended rate constants than contained in this table, but it does contain most of those which are applicable to atmospheric chemistry. Evaluations and compilations of rate data and on-going programs in these areas have been described in the recent review paper "Evaluation and Compilation of Reaction Rate Data" by R. F. Hampson and D. Garvin, Journal of Physical Chemistry 81, 2317-2319 (1977). A current extensive listing of sources of evaluated rate data, NBS List of Publications 73 "Chemical Kinetics Tables, Data Evaluations and Bibliographies. A Guide to the Literature" is available on request from the NBS Chemical Kinetics Information Center.

Three sets of detailed data sheets have been published by us in the course of preparing these tables. They are R. F. Hampson (editor) "Survey of Photochemical and Rate Data for Twenty-eight Reactions of Interest in Atmospheric Chemistry" J. Phys. Chem. Ref. Data 2, 267 (1973);

R. F. Hampson (editor) "Chemical Kinetics Data Survey VI, NBSIR 73-207 (1973); and D. Garvin (editor) "Chemical Kinetics Data Survey V" NBSIR 73-206 (1973), all recommendations contained in them (and still pertinent) are summarized in the present table.

We have also accepted many recommendations made by R. T. Watson in "Rate Constants for Reactions of  $\text{ClO}_x$  of Atmospheric Interest"

J. Phys. Chem. Ref. Data 6, 871 (1977) and by D. L. Baulch, et al "Evaluated Kinetic Data for High Temperature Reactions" Volume 1 (1972), Volume 2 (1973) and Volume 3 (1976), Butterworth and Co., London.

In addition to recommendations on rate and photochemical data the table includes listings of current research results. These data listings serve several purposes. Some simply record measurements, usually limited in number, on reactions for which it is not yet practical to give recommended values. Others show the data upon which a new recommendation is based. Still others show what has been done on a reaction since its rate constant was last evaluated. These new data may support the recommendation or suggest the need for modifications in the future.

## 2. Guide to the Table

### 2.1 General

This table provides current (December 1977) information on reaction rate constants, quantum yields and absorption cross sections. For many reactions, preferred values are given. The reactions included in the table are summarized in the index of reactions given in section 3.

Most of the important stratospheric reactions are in the tables. A number of the less important ones and some related systems are included, often simply for comparison.

The following remarks summarize the content of the table. It lists 416 reactions and gives a preferred value of the rate constant for 194 reactions; 136 based on recent reviews and 58 based on recent (1975-1977) experimental work. New data entries (1975-1977) are given for 252 reactions, showing substantial activity in the study of gas kinetics.

The following principles have been used in the selection and presentation of data:

- a. Where a preferred value is given for a rate constant or photochemical quantity, it is so indicated by an asterisk [\*] placed ahead of the entry in the reference column.
- b. As indicated earlier an asterisk preceded by a dagger symbol [†\*] is used to indicate those preferred values that have been recommended by the NASA Laboratory Measurements Committee and published in NASA Reference Publication 1010 "Chlorofluoromethanes and the Stratosphere" R. D. Hudson, editor, August 1977.



- c. Where there is a recent published evaluation of the data and there are no newer data, the evaluation is adopted and usually marked with an asterisk. The original data covered by the evaluation are not listed separately. However this latter rule has not been applied when the evaluation has appeared within the past year.
- d. Where there is an evaluation but there are new data, both are listed and a preferred value is indicated (marked by an asterisk).
- e. Where desirable, the available recent data sets are listed, and a selection is made or a preferred value is synthesized from them.

## 2.2 Uncertainty in Recommended Value of a Rate Constant

The uncertainty assigned here to the recommended value of a rate constant is given in the column "Notes and reliability of log k". This is an estimate by the evaluator of the absolute accuracy of the preferred value. It is a subjective judgment derived from intercomparison of data sets, consideration of related reactions studied with the same technique, estimates of how well the parameters could have been controlled, and comparison with theory. It means that in the evaluators judgment, the true value will lie within the indicated limits to a high level of confidence (90 to 95 percent).

Usually the uncertainty is indicated by the term  $D$  in the expression:  $\log_{10} k = C \pm D$ . This is equivalent to the statement that  $k$  is uncertain to a factor of  $F$  where  $D = \log_{10} F$ . The statement that  $k$  has the value  $k_0$  and is uncertain to a factor of  $F$  means that  $k_0/F < k < k_0 F$ .

Other forms used to indicate reliability are the following:

$A < k < B$  means  $k$  lies in the range between  $A$  and  $B$   
 $k < (>) B$  means  $B$  is an upper (lower) limit  
 $k \sim B$  means  $B$  is only a rough guide to value of  $k$   
 $k = A \pm B$  alternative form for stating reliability limits

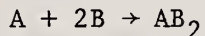
At times a rate constant expression is quoted from a paper with individual uncertainties for the rate parameters as  $k = (A \pm a) \exp(-B \pm b/T)$ . These measures are those provided by the author and often are indications of precision, not overall reliability.

Some notes are in order, regarding the statement of the uncertainty in the recommended value of the rate constant for those recommended values recommended by the NASA Laboratory Measurements Committee. Those recommendations were made for the limited temperature range 200-300 K. The uncertainty is indicated for  $T = 230$  K, a typical midstratospheric temperature and in some cases allowance for extrapolation from higher temperatures was necessary. This is why occasionally the entry consists of the value of a rate constant measured at 298 K, the symbols [<sup>†</sup>\*] immediately ahead of the entry in the reference column to show that this value has been adopted by the Committee for the temperature range 200-300 K, and a statement of the uncertainty in the preferred value at  $T = 230$  K. This stated uncertainty will generally be larger than the uncertainty in the measured value (measured at 298 K) to allow for the additional uncertainty introduced by extrapolation to  $T = 230$  K.

For the recommendations made by the NASA Laboratory Committee the indicated uncertainties in NASA Reference Publication 1010 have been doubled in the present table in order to make the reliability statement analogous to a "95 percent confidence level".

### 2.3 Conventions Concerning Rate Constants

a. General Convention. Almost all of the reactions in the table are elementary processes. For them the rate expression is derivable from a statement of the reaction, e.g.

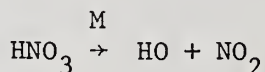
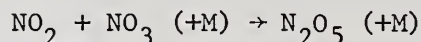


$$-d[A]/dt = -(1/2) d[B]/dt = d[AB_2]/dt = k[A][B]^2$$

Note that the stoichiometric coefficient for B, i.e. 2, appears in the denominator before B's rate of change (which is equal to  $2k[A][B]^2$ ) and as a power on the right hand side.

Wherever there may be any doubt an explicit rate expression is given.

b. Dissociation and Combination Reactions. Some reactions of these types are not of integral kinetic order over the stratospheric pressure and temperature range. That is, although they require an energy transfer agent, "M," they are in the "pressure fall-off region". For some such reactions we tabulate rate constants that include the effect of the energy transfer agent and give rates for various altitudes. The reactions are written to demphasize "M," e.g.,



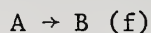
The rate expressions to be used do not have the concentration of M in them, e.g., Rate =  $k[\text{NO}_2][\text{NO}_3]$  and  $k[\text{HNO}_3]$  respectively. The units given for the k's, s<sup>-1</sup> for first order, and cm<sup>+3</sup> molecule<sup>-1</sup>s<sup>-1</sup> for second order, are consistent with this convention.

The altitude, temperature and number density regime used in these cases is

altitude/km	temp./K	log[M]/molecule cm <sup>-3</sup>
15	217	18.60
20	217	18.27
25	222	17.93
30	227	17.58
35	237	17.26
40	251	16.92
45	265	16.60

This table follows the U. S. standard atmosphere, 1976.

c. Forward and Reverse Reactions. In some cases there are no data on a reaction of interest but there are data on the "reverse" reaction. Occasionally, for



an evaluation will use the data on the "reverse" reaction together with an equilibrium constant to obtain the other rate constant. Obviously this is an approximation but it often is a useful method of estimating non-measured physical properties.

The table contains notations to warn the reader when this procedure has been used, such as "based on reverse reaction," or when both reactions  $f$  and  $r$  are listed together " $k_f = k_r K_{eq}$ " or  $k_r = k_f / K_{eq}$ . These expressions, which are those used in the analyses, are based on equating the two rates at equilibrium.

$$R_f = R_r$$

$$k_f[A] = k_r[B]$$

$$K_{eq} = [B]/[A] = k_f/k_r.$$

## 2.4 Convention Concerning Optical Absorption Coefficients

These are reported in the table as "absorption cross sections per molecule, base e". They are defined by the equations.

$$I/I_0 = \exp(-\sigma[N]\ell)$$

$$\sigma = (1/([N]\ell)) \ln(I_0/I)$$

where  $I_0$  and  $I$  are the intensities of incident and transmitted light,  $\sigma$  is the absorption cross section,  $\text{cm}^2\text{molecule}^{-1}$ ,  $[N]$  is the concentration of absorbers,  $\text{molecules cm}^{-3}$ , and  $\ell$  is the path length, cm. Other definitions and units are frequently used. The terms "absorption coefficient" and "extinction coefficient" are common. It is always necessary to know what concentration units, path length units and type of logarithm (base e or base 10) are used in the definition. To convert "cross-sections" to absorption coefficients in  $(\text{atm at } 273 \text{ K})^{-1} \text{ cm}^{-1}$ , base e, multiply by  $2.69 \times 10^{19}$ .

A table of conversion factors is given in the appendix.



### 3. Arrangement of the Table

Data on a reaction appear only once in the table. The normal location for a reaction is determined by its reactants. Each species has been assigned a sequence number (1 to 65) as shown in the index that follows. These sequence numbers are the same as those used in NBS Technical Note 866. New species have been inserted in appropriate positions and assigned sequence numbers such as 34a, 34b, etc. A reaction is filed under the lower numbered species. That is, the reaction of ozone (7) with an oxygen atom (1) is filed under reactions of oxygen atoms. The numbers for the reactants appear at the left margin of the table, preceding the statement of the reaction, e.g. 1,7  $O + O_3 \rightarrow O_2 + O_2$ . These number pairs run in ascending order through the table.

If a reaction is not filed in the location described above, a cross reference is given there. The most common exception is the listing together of data on the forward and reverse reactions of a pair, i.e.  $A \rightarrow B$ ,  $B \rightarrow A$ .

In the index that follows, bimolecular reactions are listed under both reactants. Frequently the listing of reaction partners for a particular species is divided into two parts by three dashes, separating species earlier in the list than the species indexed from those later in the list. Reactions of the particular species with those species listed before the three dashes should be sought under those reaction partners. There is no indexing of products of reactions. A few species are listed in the index for which there are no reactions in the table, in anticipation of expansion of the data set.

# REACTION INDEX

1. O                    Rxn with: O, O(<sup>1</sup>S), O<sub>2</sub>, O<sub>3</sub>, N, NO, NO<sub>2</sub>, NO<sub>3</sub>, N<sub>2</sub>, N<sub>2</sub>O, N<sub>2</sub>O<sub>5</sub>, NH<sub>2</sub>, NH<sub>3</sub>, H, HO, HO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>, HNO<sub>2</sub>, HNO<sub>3</sub>, SO, SO<sub>2</sub>, SO<sub>3</sub>, HS, H<sub>2</sub>S, CS, CS<sub>2</sub>, OCS, ClO, BrO, OClO, HCl, HBr, NO<sub>3</sub>Cl, Cl<sub>2</sub>, Cl<sub>2</sub>O, CO, CO<sub>2</sub>, CN, CHO, CH<sub>2</sub>O, CH<sub>3</sub>, CH<sub>3</sub>NO<sub>2</sub>, CH<sub>3</sub>ONO, CH<sub>4</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>6</sub>, alkane, C<sub>6</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub>, CH<sub>3</sub>Cl
  
2. O(<sup>1</sup>D)                Rxn with: O<sub>2</sub>, O<sub>3</sub>, NO, NO<sub>2</sub>, N<sub>2</sub>, N<sub>2</sub>O, NH<sub>3</sub>, H<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>, HCl, CO<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, CF<sub>2</sub>Cl<sub>2</sub>, CFC1<sub>3</sub>
  
3. O(<sup>1</sup>S)                Rxn with: O, O<sub>2</sub>, O<sub>3</sub>, NO, NO<sub>2</sub>, N<sub>2</sub>, N<sub>2</sub>O, NH<sub>3</sub>, H<sub>2</sub>O, CO<sub>2</sub>, CH<sub>4</sub>
  
4. O<sub>2</sub>                   Rxn with: O, O(<sup>1</sup>D), O(<sup>1</sup>S) - - -  
                               hv, N, NO, NO<sub>2</sub>, NO<sub>3</sub>, N<sub>2</sub>, H, H<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>, HNO, SO, HS, Cl, CN, CHO, CH<sub>3</sub>, CH<sub>3</sub>O
  
5. O<sub>2</sub>(<sup>1</sup>Δ)              Rxn with: O<sub>2</sub>, O<sub>3</sub>, N, NO, N<sub>2</sub>, H, SO, SO<sub>2</sub>, H<sub>2</sub>S, CO, CF<sub>2</sub>Cl<sub>2</sub>, CCl<sub>4</sub>, CH<sub>3</sub>Cl, CH<sub>2</sub>Cl<sub>2</sub>, CHCl<sub>3</sub>
  
6. O<sub>2</sub>(<sup>1</sup>Σ)              Rxn with: O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O
  
7. O<sub>3</sub>                   Rxn with: O, O(<sup>1</sup>D), O(<sup>1</sup>S), O<sub>2</sub>(<sup>1</sup>Δ) - - -  
                               hv, M, N, NO, NO<sub>2</sub>, H, HO, HO<sub>2</sub>, SO, SO<sub>2</sub>, H<sub>2</sub>S, Cl, Br, ClO, BrO, CO, CH<sub>2</sub>O, CH<sub>3</sub>, CH<sub>3</sub>O<sub>2</sub>, CH<sub>3</sub>ONO, CH<sub>4</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>3</sub>H<sub>6</sub>, allene, butenes, butadiene, C<sub>2</sub>Cl<sub>2</sub>H<sub>2</sub>

8. N                    Rxn with: O, O<sub>2</sub>, O<sub>2</sub>(<sup>1</sup>Δ), O<sub>3</sub> - - -  
N, NO, NO<sub>2</sub>, HO, SO, SO<sub>3</sub>, OC1O
  
9. NO                   Rxn with: O, O(<sup>1</sup>D), O(<sup>1</sup>S), O<sub>2</sub>, O<sub>2</sub>(<sup>1</sup>Δ), O<sub>3</sub>, N - - -  
hv, M, NO, NO<sub>2</sub> + H<sub>2</sub>O, NO<sub>3</sub>, NH, NH<sub>2</sub>, H, HO,  
HO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>, Cl, ClO, BrO, OC1O,  
CH<sub>3</sub>, CH<sub>3</sub>O, CH<sub>3</sub>O<sub>2</sub>
  
10. NO<sub>2</sub>                Rxn with: O, O(<sup>1</sup>D), O(<sup>1</sup>S), O<sub>2</sub>, O<sub>3</sub>, N, NO + H<sub>2</sub>O - - -  
hv, M, NO<sub>2</sub>, NO<sub>3</sub>, NH<sub>2</sub>, NH<sub>3</sub>, H, HO, HO<sub>2</sub>,  
SO<sub>2</sub>, Cl, ClO, CH<sub>3</sub>, CH<sub>3</sub>O, CH<sub>3</sub>O<sub>2</sub>
  
11. NO<sub>3</sub>                Rxn with: O, O<sub>2</sub>, NO, NO<sub>2</sub> - - -  
hv, M, NO<sub>3</sub>, H<sub>2</sub>O, SO<sub>2</sub>
  
12. N<sub>2</sub>                   Rxn with: O, O(<sup>1</sup>D), O(<sup>1</sup>S), O<sub>2</sub>, O<sub>2</sub>(<sup>1</sup>Δ), O<sub>2</sub>(<sup>1</sup>Σ) - - -  
M, HO
  
13. N<sub>2</sub>O                Rxn with: O, O(<sup>1</sup>D), O(<sup>1</sup>S) - - -  
hv, M, H, HO, ClO, CO
  
14. N<sub>2</sub>O<sub>5</sub>              Rxn with: O - - - hv, M, H<sub>2</sub>O, SO<sub>2</sub>
  
15. NH                   Rxn with: NO - - -
  
16. NH<sub>2</sub>                Rxn with: O, NO - - - H, HO, H<sub>2</sub>, H<sub>2</sub>O
  
17. NH<sub>3</sub>                Rxn with: O, O(<sup>1</sup>D), O(<sup>1</sup>S), NO<sub>2</sub> - - -  
M, H, HO, ClO



- 17a.  $N_2H_4$       Rxn with: H
18. H      Rxn with:  $O$ ,  $O_2$ ,  $O_2(^1\Delta)$ ,  $O_3$ , NO,  $NO_2$ ,  $N_2O$ ,  $NH_2$ ,  $NH_3$ ,  
 $N_2H_4$  - - -  
H, HO,  $HO_2$ ,  $H_2O$ ,  $H_2O_2$ , HNO,  $HNO_2$ ,  $HNO_3$ ,  
 $SO_2$ , HS,  $H_2S$ , COS, OClO, HCl, NOCl,  $Cl_2$ , CO,  
 $CO_2$ ,  $CH_2O$ ,  $CH_3OOH$ ,  $CH_3ONO$ ,  $CH_3Cl$
19. HO      Rxn with:  $O$ ,  $O_3$ , N, NO,  $NO_2$ ,  $N_2$ ,  $N_2O$ ,  $NH_2$ ,  $NH_3$ , H - - -  
M, HO,  $HO_2$ ,  $H_2$ ,  $D_2$ ,  $H_2O$ ,  $H_2O_2$ , HNO,  $HNO_2$ ,  
 $HNO_3$ ,  $SO_2$ ,  $H_2S$ , Cl, HCl, DCl, HBr,  $NO_3Cl$ ,  
CO,  $CH_2O$ ,  $CH_3OH$ ,  $CH_3NO_2$ ,  $CH_3ONO$ ,  $CH_4$ ,  $C_2H_2$ ,  
 $C_2H_4$ ,  $C_2H_6$ ,  $C_3H_6$ ,  $C_4H_{10}$ , alkane,  $C_6H_6$ ,  
 $C_6H_5CH_3$ ,  $CF_2Cl_2$ ,  $CFCl_3$ ,  $CCl_4$ ,  $CH_3Cl$ ,  
 $CH_2Cl_2$ ,  $CHCl_3$ ,  $CH_iCl_jF_k$
20.  $HO_2$       Rxn with:  $O$ ,  $O_3$ , NO,  $NO_2$ , H, HO - - -  
M,  $HO_2$ ,  $H_2$ ,  $H_2O$ ,  $SO_2$ , Cl, Br, ClO, CO,  $CH_2O$ ,  
 $CH_3O_2$ ,  $C_2H_4$ ,  $C_2H_6$ ,  $C_3H_8$ ,  $C_4H_{10}$
21.  $H_2$       Rxn with:  $O$ ,  $O(^1D)$ ,  $O_2$ , NO,  $NH_2$ , HO,  $HO_2$  - - -  
M, Cl, ClO
22.  $H_2O$       Rxn with:  $O$ ,  $O(^1D)$ ,  $O(^1S)$ ,  $O_2$ ,  $O_2(^1\Sigma)$ , NO,  $NO_3$ ,  $N_2O_5$ ,  
 $NH_2$ , H, HO,  $HO_2$  - - -  $SO_3$
23.  $H_2O_2$       Rxn with:  $O$ ,  $O(^1D)$ ,  $O_2$ , NO, H, HO - - -  
 $h\nu$ , M, Cl, Br

24.	HNO	Rxn with: $O_2$ , H, HO - - - M, HNO
25.	HNO <sub>2</sub>	Rxn with: O, H, HO - - - hv
26.	HNO <sub>3</sub>	Rxn with: O, H, HO - - - hv, M, Cl
26a.	S	Rxn with: CS <sub>2</sub> , COS
27.	SO	Rxn with: O, O <sub>2</sub> , O <sub>2</sub> ( <sup>1</sup> Δ), O <sub>3</sub> , N - - - SO, SO <sub>3</sub>
28.	SO <sub>2</sub>	Rxn with: O, O <sub>2</sub> ( <sup>1</sup> Δ), O <sub>3</sub> , NO <sub>2</sub> , NO <sub>3</sub> , N <sub>2</sub> O <sub>5</sub> , H, HO, HO <sub>2</sub> - - - CH <sub>3</sub>
29.	SO <sub>3</sub>	Rxn with: O, N, H <sub>2</sub> O, SO - - -
30.	S <sub>2</sub> O	Rxn with: .
31.	HS	Rxn with: O, O <sub>2</sub> , H - - - HS
32.	H <sub>2</sub> S	Rxn with: O, O <sub>2</sub> ( <sup>1</sup> Δ), O <sub>3</sub> , H, HO - - -
33.	HSO <sub>3</sub>	Rxn with:
34.	H <sub>2</sub> SO <sub>4</sub>	Rxn with:
34a.	CS	Rxn with: O - - -
34b.	CS <sub>2</sub>	Rxn with: O, S - - -
34c.	COS	Rxn with: O, H, S - - -

35. Cl Rxn with:  $O_2$ ,  $O_3$ , NO,  $NO_2$ , HO,  $HO_2$ ,  $H_2$ ,  $H_2O_2$ ,  
 $HNO_3$  - - - Cl,  $ClO$ ,  $ClOO$ ,  $NOCl$ ,  $NO_2Cl$ ,  
 $NO_3Cl$ ,  $Cl_2O$ ,  $CH_4$ ,  $C_2H_6$
- Br Rxn with:  $O_3$ ,  $HO_2$ ,  $H_2O_2$  - - -
36.  $ClO$  Rxn with:  $O$ ,  $O_3$ , NO,  $NO_2$ ,  $N_2O$ ,  $NH_3$ ,  $HO_2$ ,  $H_2$  - - -  
 $h\nu$ ,  $ClO$ ,  $BrO$ , CO,  $CH_4$ ,  $C_2H_2$ ,  $C_2H_4$
- BrO Rxn with:  $O$ ,  $O_3$ , NO,  $ClO$  - - - BrO
37.  $ClOO$  Rxn with: Cl - - -  $h\nu$ , M
- $OCIO$  Rxn with:  $O$ , N, NO, H, Cl - - -  $h\nu$
38.  $ClO_3$  Rxn with:
39. HCl Rxn with:  $O$ ,  $O(^1D)$ , H, HO - - -  $h\nu$
- HBr Rxn with:  $O$ , HO - - -
40.  $HOCl$  Rxn with:  $h\nu$
41.  $HOClO$  Rxn with:
42.  $NOCl$  Rxn with: H, Cl - - -  $h\nu$
43.  $NO_2Cl$  Rxn with: Cl - - -  $h\nu$
- 43a.  $NO_3Cl$  Rxn with:  $O$ , HO, Cl - - -  $h\nu$
44.  $Cl_2$  Rxn with:  $O$ , H - - -  $h\nu$
- 44a.  $Cl_2O$  Rxn with:  $O$ , Cl - - -

45.	CO	Rxn with: O, O <sub>2</sub> ( <sup>1</sup> Δ), O <sub>3</sub> , N <sub>2</sub> O, H, HO, HO <sub>2</sub> , ClO - - - CH <sub>3</sub> O
46.	CO <sub>2</sub>	Rxn with: O, O( <sup>1</sup> D), O( <sup>1</sup> S), H - - - M
46a.	CN	Rxn with: O, O <sub>2</sub> - - -
47.	CHO	Rxn with: O, O <sub>2</sub> - - -
48.	CH <sub>2</sub> O	Rxn with: O, O <sub>3</sub> , H, HO, HO <sub>2</sub> - - - hν
49.	CH <sub>3</sub>	Rxn with: O, O <sub>2</sub> , O <sub>3</sub> , NO, NO <sub>2</sub> , SO <sub>2</sub> - - -
50.	CH <sub>3</sub> O	Rxn with: O <sub>2</sub> , NO, NO <sub>2</sub> , CO
51.	CH <sub>3</sub> O <sub>2</sub>	Rxn with: O <sub>3</sub> , NO, NO <sub>2</sub> , HO <sub>2</sub> - - - CH <sub>3</sub> O <sub>2</sub>
52.	CH <sub>3</sub> OH	Rxn with: HO - - -
53.	CH <sub>3</sub> OOH	Rxn with: H - - -
54.	CH <sub>3</sub> NO <sub>2</sub>	Rxn with: O, HO - - -
	CH <sub>3</sub> ONO	Rxn with: O, O <sub>3</sub> , H, HO - - - hν
55.	CH <sub>3</sub> NO <sub>3</sub>	Rxn with:
56.	CH <sub>4</sub>	Rxn with: O, O( <sup>1</sup> D), O( <sup>1</sup> S), O <sub>3</sub> , HO, Cl, ClO - - -
56a.	C <sub>2</sub> H <sub>2</sub>	Rxn with: HO, ClO - - -
57.	C <sub>2</sub> H <sub>4</sub>	Rxn with: O, O <sub>3</sub> , HO, HO <sub>2</sub> , ClO - - -

58.  $C_2H_6$  Rxn with:  $O$ ,  $O(^1D)$ ,  $HO$ ,  $HO_2$ ,  $Cl$  - - -
- \*59.  $C_3H_6$  Rxn with:  $O$ ,  $O_3$ ,  $HO$  - - -
- +60.  $C_3H_8$  Rxn with:  $O$ ,  $HO$ ,  $HO_2$  - - -
- ∇60a.  $C_6H_6$  Rxn with:  $O$ ,  $HO$  - - -
61.  $CF_2Cl_2$  Rxn with:  $O(^1D)$ ,  $O_2(^1\Delta)$ ,  $HO$  - - -  $h\nu$
62.  $CFC1_3$  Rxn with:  $O(^1D)$ ,  $HO$  - - -  $h\nu$
63.  $CCl_4$  Rxn with:  $HO$  - - -  $h\nu$
64.  $CH_iCl_j$  Rxn with:  $O$ ,  $O_2(^1\Delta)$ ,  $O_3$ ,  $H$ ,  $HO$  - - -
- √65.  $CH_iCl_jF_k$  Rxn with:  $HO$  - - -

\* and higher alkenes  
 † and higher alkanes  
 ∇ and other aromatics  
 √ and other halocarbons

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
1.1M	$\phi + \phi + M \rightarrow \phi_2 + M$ *Campbell, Gray (1973)	298	$4.8 \times 10^{-33}$	M = N <sub>2</sub> ±0.03
		196	$11.1 \times 10^{-33}$	±0.02
	*Johnston (1968) review	1000-8000	$3.80 \times 10^{-30} T^{-1} \exp(-170/T)$	M = O <sub>2</sub> ±0.3
	Taylor (1975) review	2000-10000	$1.7 \times 10^{-32} T^{-1/2}$	M = N <sub>2</sub>
			$2.2 \times 10^{-28} T^{-3/2}$	M = O <sub>2</sub>
			$6.2 \times 10^{-28} T^{-3/2}$	M = O
			$8.3 \times 10^{-33} T^{-1/2}$	M = N, N <sup>+</sup>
			$5.2 \times 10^{-35} \exp(900/T)$	M = Ar ±0.1 at 190K
1.3	Baulch, et al (1976) review	190-4000	see O(1S) + O →	
1.4M	$O(^1P) + \phi_2 + M \rightarrow \phi_3 + M$ (f)			
7,M	$\phi_3 + M \rightarrow \phi + \phi_2 + M$ (r)			
	*This Survey			
		200-346	$k_f = 6.6 \times 10^{-35} \exp(510/T)$	M = Ar ±0.7
			Rel. M eff.: Ar(1.0), N <sub>2</sub> (1.6), O <sub>2</sub> (1.7), H <sub>2</sub> O(15)	
		300	$k_f = 5.5 \times 10^{-34}$	M = N <sub>2</sub>
	Baulch, et al (1976) review	200-1000	$k_r = 4.1 \times 10^{-10} \exp(-11430/T)$	M = Ar
		200-1000	$k_f = 4.6 \times 10^{-35} \exp(1050/T)$	M = O <sub>2</sub> ±0.1
	Johnston (1968) eval.		$k_r = 1.65 \times 10^{-9} \exp(-11400/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	±0.1
			Rel. M eff.: O <sub>3</sub> (1.0), Ar(0.25), O <sub>2</sub> (0.44), N <sub>2</sub> (0.30)	
	Hule, Herron, Davis (1972)	200-346	$k_f = 6.6 \times 10^{-35} \exp(510/T)$	M = Ar
			Rel. M efficiencies: Ar(1.0), He(0.9), N <sub>2</sub> (1.7)	
	Mulcahy, Williams (1968)	213-386	$k_f = 4.7 \times 10^{-35} \exp(840/T)$	M = Ar
			Rel. M eff.: Ar(1.0), He(0.8), CO <sub>2</sub> (3.4), O <sub>2</sub> (1.1)	
	Meaburn, et al (1968)	300	$k_f = 1.0 \times 10^{-33}$	M = CO <sub>2</sub>
			Rel. M eff.: CO <sub>2</sub> (1.0), C <sub>6</sub> H <sub>6</sub> (0.44), N <sub>2</sub> O(0.88)	
	Stuhl, Niki (1971)	300	$k_f = 5.4 \times 10^{-34} \text{ cm}^6 \text{ molecule}^{-2} \text{ s}^{-1}$	M = N <sub>2</sub>
			Rel. M efficiencies: N <sub>2</sub> (1.0), O <sub>2</sub> (1.18), C <sub>6</sub> H <sub>6</sub> (1.24)	
	Donovan, Husain, Kirsch (1970)	300	$k_f = 5.0 \times 10^{-34} \text{ cm}^6 \text{ molecule}^{-2} \text{ s}^{-1}$	M = Ar
			Rel. M efficiencies: Ar(1.0), Kr(0.98), He(0.92)	
			$k_f = 8 \times 10^{-34}$	M = N <sub>2</sub>
	Hippler, Troe (1971)	300	$k_f = 4.4 \times 10^{-34}$	M = Ar, Rel. eff. Ar(1.0), N <sub>2</sub> (1.6)
	Slanger, Black (1970)	300	$k_f = 1.24 \times 10^{-34}$	M = O <sub>2</sub>
	Francis (1969)	300	$k_f = 2.28 \times 10^{-34}$	M = Ar
	Sauer (1967)	300	$k_f = 5.4 \pm 1.2 \times 10^{-34}$	M = N <sub>2</sub>
	Ball and Larkin (1973)	295	Rel. efficiencies: N <sub>2</sub> (1.0), O <sub>2</sub> (1.09), Ar(0.78)	
			$k_f \sim 8 \times 10^{-34} \text{ cm}^6 \text{ molecule}^{-2} \text{ s}^{-1}$	M = N <sub>2</sub> (a)
	Hippler, Schippert, Troe (1975)	300	$k_f(\infty) = 2.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	(a,b)

[illegible]





No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of $\log k$
<b>Hippler, Schippert, Troe (1975)</b>				
1,11	$\text{O} + \text{NO}_3 \rightarrow \text{O}_2 + \text{NO}_2$	300	$k_r \sim 8 \times 10^{-42} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}$ , $M = \text{N}_2$	(a)
1,12	Graham, Johnston (1978)		$k_f = 8.0 \times 10^{-32} \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ , $M = \text{N}_2$	(b)
1,12M	$\text{O} + \text{N}_2 \rightarrow \text{N} + \text{NO}$		$k_f(\text{a}) = 2.0 \times 10^{-11} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}$	
13,M	$\text{N}_2\text{O} + \text{M} \rightarrow \text{N}_2 + \text{O} + \text{M}$ (r)		(a) No reliable data. Value based on $k_f$	
	Baulch, et al (1973) review		(b) 2d order high pressure limit	
		1300-2500	$k_f = 3.9 \times 10^{-35} \exp(-10400/T) \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$	
			$\text{M} = \text{Ar}$	
			$k_r = 8.3 \times 10^{-10} \exp(-29000/T) \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}$	$\pm 0.2$ (a)
		900-2100	$\text{M} = \text{Ar}$	
			$k_f = 5.5 \times 10^{-15} \exp(-11330/T) \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}$	$\pm 0.2$
			$k_r = 1.3 \times 10^{-11} \exp(-30000/T)\text{s}^{-1}$	$\pm 0.2$ (a,b)
			(a) $k_f = k_r K_{\text{eq}}$	$\pm 0.2$ (c)
			(b) 2d order high pressure limit	
			(c) 1st order high pressure limit	
	Schofield (1973) review	300-568	$k_f \leq 5 \times 10^{-38} \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$	upper limit only
		800-2100	$k_r = 1.4 \times 10^{11} \exp(-30,000/T)\text{s}^{-1}$	1st order limit
1,13	$\text{O} + \text{N}_2\text{O} \rightarrow \text{N}_2 + \text{O}_2$ (1)			
1,13	$\text{O} + \text{N}_2\text{O} \rightarrow \text{NO} + \text{NO}$ (2)			
9,9	$\text{NO} + \text{NO} \rightarrow \text{N}_2\text{O} + \text{O}$ (2r)			
	Baulch, et al (1973) review			
		1200-2000	$k_1 = 1.7 \times 10^{-10} \exp(-14.1 \times 10^3/T)$	$\pm 0.4$ (a)
			$k_2 = 1.7 \times 10^{-10} \exp(-14.1 \times 10^3/T)$	$\pm 0.3$
		1200-2000	$k_{2r} = 2.2 \times 10^{-12} \exp(-32100/T)$	$\pm 0.7$ (b)
			(a) Based on $k_1/k_2 = 1$	
			(b) $d[\text{NO}]/dt = -2k_{2r}[\text{NO}]^2$	
	Taylor (1975) review	2000-10000	$k_{2r} = 0.4T^{5/2} \exp(-43000/T)$	
1,14	$\text{O} + \text{N}_2\text{O}_5 \rightarrow \text{products}$			
	Graham, Johnston (1978)	300	$< 2 \times 10^{-14}$	preliminary
	Davis (1974)	300	$< 2 \times 10^{-13}$	
1,16	$\text{O} + \text{NH}_2 \rightarrow \text{HN} + \text{H}$ (a)			
	$\rightarrow \text{HO} + \text{NH}$ (b)			
	Gehring, et al (1973)	300	$3.5 \times 10^{-12} (k_a + k_b)$	
1,17	$\text{O} + \text{NH}_3 \rightarrow \text{HO} + \text{NH}_2$ (f)			
16,19	$\text{HO} + \text{NH}_2 \rightarrow \text{O} + \text{NH}_3$ (r)			
	*Kurylo, et al (1969)			
	Baulch, et al (1973) review	361-677	$k_f = 6.6 \times 10^{-12} \exp(-3300/T)$	$\pm 0.3$
		300-1000	$k_f = 2.5 \times 10^{-12} \exp(-3020/T)$	$\pm 0.2$
		300-1000	$k_r = k_f/K_{\text{eq}} = 1 \times 10^{-13}$	$\pm 0.2$ (a)

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k
1.18M	Albers, et al (1965) Kondratiev (1970) review	300-1000 350-1000	$k_f = 2 \times 10^{-12} \exp(-3000/T)$ $k_r = 1.8 \times 10^{-12} \exp(-2500/T)$ Data of Albers, et al provide an upper limit when extrapolated to 220K (a) $\text{H}\theta + \text{NH}_2 \rightarrow \text{NH} + \text{H}_2\theta$ may be preferred channel.	
1.19 4.18	$\theta + \text{H} + \text{M} \rightarrow \text{H}\theta + \text{M}$ Schofield (1973) review Baulch, et al (1972) review $\theta + \text{H}\theta \rightarrow \text{H} + \theta_2$ (f) $\theta_2 + \text{H} \rightarrow \theta + \text{H}\theta$ (r)	1000-3000	$\sim 2 \times 10^{-32} \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ M = Ar No recommendation	$\pm 1$ estimate
1.19M 20,M	†*Wilson (1972) review †Baulch, et al (1972) review Baulch, et al (1972) review $\theta + \text{H}\theta + \text{M} \rightarrow \text{H}\theta_2 + \text{M}$ (f) $\text{H}\theta_2 + \text{M} \rightarrow \theta + \text{H}\theta + \text{M}$ (r)	300-2000 700-2500 300	$k_f = 4.2 \pm 1.7 \times 10^{-11}$ $k_r = 3.7 \times 10^{-10} \exp(-8450/T)$ $k_f = 3.8 \pm 1.7 \times 10^{-11}$	$\pm 0.3$ $\pm 0.1$ $\pm 0.17$
1.20	Baulch, et al (1972) review $\theta + \text{H}\theta_2 \rightarrow \text{H}\theta + \theta_2$ †*Burrows, Harris, Thrush (1977)	293	no recommendation for forward or reverse rxn $3.5 \times 10^{-11}$ (a) Based on value for $k(\theta + \text{H}\theta)$ and $k(\text{H}\theta + \text{H}_2\theta_2)$	$\pm 0.3$ at 230K (a)
1.21 18,19	Lloyd (1974) review $\theta + \text{H}_2 \rightarrow \text{H}\theta + \text{H}$ (f) $\text{H} + \text{H}\theta \rightarrow \theta + \text{H}_2$ (r) Baulch, et al (1972) review	$\sim 300$ 400-2000	$8 \times 10^{-11} \exp(-500/T)$	estimate
1.22 1.22	Dubinsky, McKenney (1975) Schott, et al (1974) Campbell, Handy (1975) $\theta + \text{H}_2\theta \rightarrow \text{H}\theta + \text{H}\theta$ $\theta + \text{H}_2\theta \rightarrow \text{H} + \text{H}\theta_2$	347-742 1400-1900 363-490	$k_f = 3.0 \times 10^{-14} (T) \exp(-4480/T)$ $k_r = k_f/K_{\text{eq}} = 1.4 \times 10^{-14} (T) \exp(-3500/T)$ $k_f = 8.8 \times 10^{-12} \exp(-4200/T)$ $k_f/k_{\text{ref}} = 3.6 \pm 0.7$ Ref rxn is $\theta_2 + \text{H} \rightarrow \theta + \text{H}\theta$ $k_f = 5.1 \times 10^{-11} \exp(-4950/T)$ See reverse reaction	$\pm 0.1$ $\pm 0.15$
1.23	Baulch, et al (1972) review $\theta(3P) + \text{H}_2\theta_2 = \text{H}\theta_2 + \theta\text{H}$ (a) $= \text{H}_2\theta + \theta_2$ (b) †*Davis, Wong, Schiff (1974) Foner, Hudson (1962) Albers, et al (1971)	283-373 300 370-800	no recommendation $k(a+b) = 2.75 \times 10^{-12} \exp(-2135/T)$ $\leq 4 \times 10^{-15}$ $k(a+b) = 4.6 \times 10^{-11} \exp(-3220/T)$ (a) Although there is no evidence, products are most likely $\theta\text{H} + \text{H}\theta_2$ as the channel to produce $\text{H}_2\theta + \theta_2$ requires a complex rearrangement.	$\pm 0.3$ (a)
1.25	$\theta + \text{HN}\theta_2 \rightarrow \text{H}\theta + \text{N}\theta_2$ This survey		No data. Probably faster than $\theta + \text{HN}\theta_3$ , since it is 94 kJ/mol more exothermic.	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of $\log k$
1,26	$\text{O} + \text{HN}\text{O}_3 \rightarrow \text{HO} + \text{NO}_3$ *Chapman, Wayne (1974) Hampson, et al (1973) review Morley, Smith (1972) Baulch, et al (1973) review	300 300 300 300	$< 3 \times 10^{-17}$ $< 1.5 \times 10^{-14}$ $< 1.3 \times 10^{-14}$ $< 10^{-14}$	
1,27	$\text{O} + \text{SO} \rightarrow \text{SO}_2 + \text{hv}$ Baulch, et al (1976) review		no recommendation	approximate upper limit
1,27M 28,M	$\text{O} + \text{SO} + \text{M} \rightarrow \text{SO}_2 + \text{M}$ (f) $\text{SO}_2 + \text{M} \rightarrow \text{O} + \text{SO} + \text{M}$ (r) *Baulch, et al (1976) review	298	$k_f = 1.9 \times 10^{-31} \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ $k_r$ no recommendation $k_f = 8.8 \times 10^{-31}$ , $\text{M} = \text{Ar}$ $k_r = 4.2 \times 10^{-10} \exp(-55000/T)$	$\text{M} = \text{Ar}$ $\pm 0.15$ $\pm 0.3$ $\pm 0.3$
1,28 4,27	$\text{O} + \text{SO}_2 \rightarrow \text{O}_2 + \text{SO}$ (f) $\text{O}_2 + \text{SO} \rightarrow \text{O} + \text{SO}_2$ (r) *Baulch, et al (1976) review	440-2100 440-2100 300	$k_f = 2.1 \times 10^{-10} T^{-0.5} \exp(-9980/T)$ $k_r = 7.5 \times 10^{-13} \exp(-3250/T)$ $k_r = < 8 \times 10^{-17}$	$\pm 0.25$ (a) $\pm 0.25$
1,28M	Breckenridge, Miller (1972) Schofield (1973) review	400-2500	$k_r = 3.0 \times 10^{-13} \exp(-2800/T)$ (a) $k_f = k_r \times K_{\text{eq}}$	$\pm 0.3$
1,29	$\text{O} + \text{SO}_2 + \text{M} \rightarrow \text{SO}_3 + \text{M}$ *Davis (1976) Schofield (1973) review	220-353 250-1000	$3.4 \times 10^{-32} \exp(-1130/T) \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ $\text{N}_2(1.0)$ , $\text{He}(1.45)$ , $\text{Ar}(1.87)$ , $\text{SO}_2(56)$ $1 \times 10^{-33} \exp(\pm 500/T) \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ $\text{M} = \text{O}_2$ , $\text{N}_2$ , $\text{Ar}$ , $\text{He}$	$\text{M} = \text{N}_2$ $\pm 0.3$ at 300K $\pm 0.6$ at other temp.
1,29	Atkinson, Pitts (1974) Westenberg, deHaas(1975d) Baulch, et al (1976) review $\text{O} + \text{SO}_3 \rightarrow \text{products}$ Westenberg, deHaas (1975c)	299-392 248-415	$9.2 \times 10^{-32} \exp(-1000/T)$ , $\text{M} = \text{N}_2\text{O}$ $1.07 \times 10^{-31} \exp(-1400/T)$ , $\text{M} = \text{He}$ Pel. eff: $\text{He}(1.0)$ , $\text{N}_2(2.4)$ , $\text{SO}_2(9.5)$ no recommendation	(a)
1,31	Schofield (1973) review Jacob, Winkler (1972) Baulch, et al (1976) review $\text{O} + \text{HS} \rightarrow \text{H} + \text{SO}$ Cupitt, Glass (1975) $\text{O} + \text{H}_2\text{S} \rightarrow \text{HO} + \text{HS}$ *Whytock, et al (1976)	1480-1550 300-500 295 263-495	$1.4 \times 10^{-31} \exp(785/T) \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ Rel. eff: $\text{He}(1.0)$ , $\text{N}_2(1.4)$ (a) Reaction $\text{O} + \text{SO}_3 + \text{M} \rightarrow \text{products}$ found to be 3rd order up to $p = 7$ Torr; $\text{SO}_4$ not detected $5 \times 10^{-10} \exp(-6000/T)$ $3 \times 10^{-16} \exp(-500/T)$ no recommendation $1.6 \pm 0.5 \times 10^{-10}$ $7.24 \times 10^{-12} \exp(-1660/T)$	uncertain        $\pm 0.1$



No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
1,34a	Hollinden, Kurylo, Timmons (1970)	205-300	2.9 x 10 <sup>-13</sup> exp(-750/T)	(a)
	Baulch, et al (1976) review		no recommendation	
	Schofield (1973) review	200-350	6.3 x 10 <sup>-13</sup> exp(-920/T)	±0.3
	δ + CS → Cδ + S		(a) Assumes stoichiometry of 3.5	
1,34b	*Baulch, et al (1976) review	300	2.2 x 10 <sup>-11</sup>	±0.2
	Bida, et al (1976)	300	2.24 x 10 <sup>-11</sup>	
	Slagle, et al (1975)	305	2.06 x 10 <sup>-11</sup>	
	δ + CS <sub>2</sub> → CS + Sδ (a) → δCS + S (b)			
1,34c	*Baulch, et al (1976) review	200-1000	k <sub>a</sub> = 3.7 x 10 <sup>-11</sup> exp(-700/T)	±0.15, T < 360K
	Wei, Timmons (1975)	218-293	k = 2.8 x 10 <sup>-11</sup> exp(-640/T)	
	Slagle, et al (1974)	302	k = 4.0 x 10 <sup>-12</sup>	
	Graham, Gutman (1976)	249-500	k <sub>b</sub> /k = 0.093 k <sub>b</sub> /k decreases from 0.098 at 249K to 0.081 at 500K	
1,36	δ + δCS → Sδ + Cδ			
	Manning, et al (1976)	296	1.10 ± 0.1 x 10 <sup>-14</sup> , P = 50 Torr 1.49 ± 0.1 x 10 <sup>-14</sup> , P = 2 torr	
	Wei, Timmons (1975)	239-404	2.0 x 10 <sup>-11</sup> exp(-2150/T)	
	Klemm, Stief (1974)	263-502	1.65 x 10 <sup>-11</sup> exp(-2165/T)	
1,36Br	Baulch, et al (1976) review	190-1200	2.6 x 10 <sup>-11</sup> exp(-2250/T)	±0.2 T < 600K ±0.5 T < 600K
	δ + Clδ → Cl + δ <sub>2</sub>			
	*NASA (1977) eval	200-300	7.7 x 10 <sup>-11</sup> exp(-130/T)	±0.12
	Clyne, Nip (1976)	220-425	1.07 x 10 <sup>-10</sup> exp(-224/T)	(a)
1,37	Zahniser, Kaufman (1977)	218-295	(a) Selected by Watson (1977) review k/k <sub>ref</sub> = (1.55±0.17)exp(246±30/T) (b) k <sub>ref</sub> = k(Cl + δ <sub>2</sub> )	(b)
	δ + Brδ → Br + δ <sub>2</sub>			
	*NASA (1977) eval	200-300	3 x 10 <sup>-11</sup>	±0.8 at 230K
	δ + δClδ → Clδ + δ <sub>2</sub>			
1,37	*NASA (1977) eval	200-300	2 x 10 <sup>-11</sup> exp(-1100/T)	±0.6 at 230K (a) ±0.2
	δ + δClδ → Clδ + δ <sub>2</sub>	298	5 x 10 <sup>-13</sup>	
	*NASA (1977) eval		(a) Based on room temp value of Bemand, et al	
	Bemand, et al (1973)			
1,39	δ + HCl → Hδ + Cl (f)			
	Hδ + Cl → δ + HCl (r)			
	*Watson (1977) eval			
	*NASA (1977) eval			
19,35	Balakhrin, et al (1971)	200-300	k <sub>f</sub> = 1.14 x 10 <sup>-11</sup> exp(-3370/T)	±0.3 at 230K
	Brown, Smith (1974)	200-300	k <sub>r</sub> = k <sub>f</sub> x K <sub>eq</sub> = 1.0 x 10 <sup>-11</sup> exp(-2970/T)	±0.3 at 230K
	Wong, Belles (1972)	295-371	k <sub>f</sub> = 1.74 ± 0.6 x 10 <sup>-12</sup> exp(-2260/T)	
	δ + HCl(v = 1) → Hδ + Cl (a) → δ + HCl(v = 0) (b)	293-440 356-628	k <sub>f</sub> = 2.5 x 10 <sup>-12</sup> exp(-2970 ± 150/T) k <sub>f</sub> = 1.9 ± 0.3 x 10 <sup>-11</sup> exp (-3580/T)	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of log k
1,39Br	Arnoldi, Wolfrum (1974) Brown, Glass, Smith (1975)	300 196-400	$3.6 \pm 1.2 \times 10^{-12}$ $6.2 \times 10^{-12} \exp(-500/T)$ (a) Total rate constant for sum of two reaction paths.	(a) (a)
1,43a	$\phi + \text{HBr} \rightarrow \text{H}\phi + \text{Br}$ †NASA (1977) eval Brown, Smith (1975) Takacs, Glass (1973) $\phi + \text{NO}_2\text{Cl} \rightarrow \text{products}$ †NASA (1977) eval Molina, et al (1977) Kurylo (1977) Ravishankara, et al (1977)	200-300 267-430 298 200-300 213-295 225-273 245	$7.6 \times 10^{-12} \exp(-1570/T)$ $4.0 \times 10^{-12} \exp(-1360 \pm 50/T)$ $(4.4 \pm 1.0) \times 10^{-14}$ $3.0 \times 10^{-12} \exp(-808/T)$ $3.4 \times 10^{-12} \exp(-840/T)$ $1.9 \times 10^{-12} \exp(-692/T)$ $2 \times 10^{-13}$ (a) Recommended expression given by Kurylo (1977) based on his work and that of Molina, et al (1977)	$\pm 0.8$ at 230K $\pm 0.15$ (a)
1,44	$\phi + \text{Cl}_2 \rightarrow \text{Cl}\phi + \text{Cl}$ *Clyne, et al (1976)	174-602	$4.2 \times 10^{-12} \exp(-1370/T)$ (a) Recommendation based on this study (299-502K) and other recent work. Also recommended by Watson (1977) review.	(a)
1,44a	$\phi + \text{Cl}_2\phi \rightarrow 2\text{Cl}\phi$ Watson (1977) review	300	$1.4 \times 10^{-11}$	$\pm 0.1$
1,45M 45M	$\phi + \text{C}\phi + \text{M} \rightarrow \text{C}\phi_2 + \text{M}$ (f) $\text{C}\phi_2 + \text{M} \rightarrow \phi + \text{C}\phi + \text{M}$ (r) *Baulch, et al (1976) review	250-500 296	$k_f = 6.5 \times 10^{-33} \exp(-2180/T)$ M = C $\phi$ $k_r = 2.3 \times 10^{-36}$ M = N $_2$ no recommendation for $k_r$	$\pm 0.2$ at 250K inc. to $\pm 0.5$ at 500K
1,46 4,45	$\phi + \text{C}\phi_2 \rightarrow \text{C}\phi + \phi_2$ (f) $\phi_2 + \text{C}\phi \rightarrow \phi + \text{C}\phi_2$ (r) *Baulch, et al (1976) review	1500-3000 1500-3000	$k_f = 2.8 \times 10^{-11} \exp(-26500/T)$ $k_r = 4.2 \times 10^{-12} \exp(-24000/T)$ (a) $k_f = k_r K_{\text{eq}}$	$\pm 0.3$ (a) $\pm 0.3$
1,46a	$\phi + \text{CN} \rightarrow \text{C}\phi + \text{N}$ Schmatjko, Wolfrum (1976)	295	$1.8 \times 10^{-11}$	
1,47	Albers, et al (1975) $\phi + \text{CH}\phi \rightarrow \text{C}\phi_2 + \text{H}$ (a) $\rightarrow \text{C}\phi + \text{H}\phi$ (b) *Washida, et al (1974) $\phi + \text{CH}_2\phi \rightarrow \text{CH}\phi + \phi\text{H}$	275-387 297	$2.0 \times 10^{-11}$ $2.1 \pm 0.4 \times 10^{-10} (k_a + k_b)$	
1,48	†NASA (1977) eval Herron, Hule (1973) review	200-300 300	$2 \times 10^{-11} \exp(-1450/T)$ $1.5 \times 10^{-13}$	$\pm 0.4$ at 230K (a) $\pm 0.15$

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
	Mack, Thrush (1973)	300	1.5 x 10 <sup>-13</sup> (a) "A factor" chosen; E <sub>act</sub> calc to fit k(300K)	±0.05
1.49	φ + CH <sub>3</sub> → CH <sub>2</sub> φ + H (a) → CHφ + Hφ (b) Washida, Bayes (1976) Washida, et al (1973) Slagle, Pruss, Gutman (1974) Morris, Niki (1972) Peeters, Mahnen (1973) Bowman (1975)	259-341 300 300 300 1100-1900 1875-2240 1550-1725	k <sub>a</sub> = 1.0 ± 0.2 x 10 <sup>-10</sup> k <sub>b</sub> negligible k <sub>b</sub> /k <sub>a</sub> < 0.05 k <sub>a</sub> = 1.85 ± 0.28 x 10 <sup>-10</sup> k <sub>a</sub> /k(φ + tetramethylethylene) = 1.5 k <sub>a</sub> = 2.2 x 10 <sup>-10</sup> exp(-1000/T) k <sub>a</sub> = 1.7 x 10 <sup>-10</sup> k <sub>a</sub> = 1.7 x 10 <sup>-10</sup>	
1.54	Biordi, et al (1975) φ + CH <sub>3</sub> NO <sub>2</sub> → products		3.3 x 10 <sup>-15</sup>	
1.54	Campbell, Goodman (1975a) φ + CH <sub>3</sub> ONO → products	295		
1.56	Davidson, Thrush (1975) φ + CH <sub>4</sub> → products	300-410	2.3 x 10 <sup>-11</sup> exp(-2620/T)	
1.57	*Herron, Huie (1973) review φ + C <sub>2</sub> H <sub>4</sub> → CH <sub>3</sub> + HCφ (a) → CH <sub>2</sub> CO + H <sub>2</sub> (b) *Herron, Huie (1973) evaluation Pruss, Slagle, Gutman (1974)	350-1000 200-500 300	3.5 x 10 <sup>-11</sup> exp (-4550/T) 5.5 x 10 <sup>-12</sup> exp (-565/T) (k <sub>a</sub> + k <sub>b</sub> ) k <sub>b</sub> = 3.81 ± 0.95 x 10 <sup>-14</sup> k <sub>b</sub> /(k <sub>a</sub> + k <sub>b</sub> ) = 0.05	±0.11 ±0.08 (a)
1.58	Atkinson, Pitts (1974) Singleton, Cvetanovic (1976)	300-392 298-486	5.6 x 10 <sup>-12</sup> exp(-640 ± 100/T) (k <sub>a</sub> + k <sub>b</sub> ) 1.16 x 10 <sup>-11</sup> exp(-845/T) a) Calculated using above recommended value for (k <sub>a</sub> + k <sub>b</sub> )	
1.59	φ + C <sub>2</sub> H <sub>6</sub> → products *Herron, Huie (1973) evaluation φ + C <sub>3</sub> H <sub>6</sub> → products	300-650	4.1 x 10 <sup>-11</sup> exp (-3200/T)	±0.11
1.60	*Herron, Huie (1973) evaluation Atkinson, Pitts (1974) Singleton, Cvetanovic (1976) φ + alkane → Hφ + alkyl radical Herron, Huie (1969)	200-500 300-392 298-483 250-600	4.1 x 10 <sup>-12</sup> exp (-38/T) 3.45 x 10 <sup>-12</sup> exp(φ ± 150/T) 1.26 x 10 <sup>-11</sup> exp(-363/T)  k = [0.8 exp(-2900/T) N <sub>p</sub> + 2.2 exp(-2250/T) N <sub>s</sub> + 2.6 exp(-1650/T) N <sub>t</sub> ] x 10 <sup>-11</sup> Where N <sub>p</sub> , N <sub>s</sub> , and N <sub>t</sub> are the number of primary, secondary, and tertiary hydrogen atoms, respectively. Do not use formula for CH <sub>4</sub> .	±0.08
1.60a	φ + C <sub>6</sub> H <sub>6</sub> → products Colussi, et al (1975) Atkinson, Pitts (1975a)	298-462 300-392	1.81 x 10 <sup>-11</sup> exp(-2115/T) 1.84 x 10 <sup>-11</sup> exp(-2000/T)	



No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of log k
1,64	$\theta + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{products}$ Colussi, et al (1975) Atkinson, Pitts (1975a) $\theta + \text{CH}_3\text{Cl} \rightarrow \text{H}\theta + \text{CH}_2\text{Cl}$ Westenberg, deHaas (1975a) Barassin, Combourieu (1974)	298-462 300-392  500-1000 298-443	$3.82 \times 10^{-11} \exp(-1940/T)$ $1.36 \times 10^{-11} \exp(-1550/T)$  $5.8 \times 10^{-11} \exp(-4550/T)$ $2.2 \times 10^{-11} \exp(-3450/T)$ (a) Also measured $k(\theta + \text{CH}_3\text{Br})/k(\theta + \text{CH}_3\text{Cl})$ to be unity over same temp. range	(a)
2,4	$\theta(^1\text{D}_2) + \theta_2 \rightarrow \theta_2(^1\Sigma_g^+) + \theta(^3\text{P})$ †Streit, et al (1976) Fletcher, Husain (1976b)	104-354 300	$2.9 \times 10^{-11} \exp(67/T)$ $5.3 \times 10^{-11}$	0.1
2,7	$\theta(^1\text{D}_2) + \theta_3 \rightarrow \theta_2 + \theta_2$ (a) $\rightarrow \theta_2 + 2\theta$ (b)	300	$k_a/k_b \sim 1$	$\pm 0.1$
2,9	†Streit, et al (1976) Heidner, et al (1973) †Cvetanovic (1975) review $\theta(^1\text{D}_2) + \text{N}\theta \rightarrow \text{N}\theta + \theta(^3\text{P})$ This survey Heidner, Husain (1973)	103-393 300 300  300 300	$2.4 \times 10^{-10} (k_a + k_b)$ $2.7 \times 10^{-10} (k_a + k_b)$ $k_a/k_b \sim 1$  $3.5 \times 10^{-11}$ $8.5 \times 10^{-11}$ (a) $0.41 \times k$ of Heidner and Husain; scaled to match other selected $\theta(^1\text{D})$ rates	$\pm 0.1$     $\pm 0.3$ (a)
2,10	$\theta(^1\text{D}_2) + \text{N}\theta_2 \rightarrow \text{N}\theta + \theta_2$ This survey Heidner, Husain (1973)	300 300	$1.0 \times 10^{-10}$ $2.3 \times 10^{-10}$ (a) $0.41 \times k$ of Heidner and Husain; scaled to match other selected $\theta(^1\text{D})$ rates	$\pm 0.2$ (a)
2,12	$\theta(^1\text{D}_2) + \text{N}_2 \rightarrow \text{N}_2 + \theta(^3\text{P})$ †Streit, et al (1976) Heidner, et al (1973) $\theta(^1\text{D}_2) + \text{N}_2 + \text{M} \rightarrow \text{N}_2\theta + \text{M}$ †NASA (1977) eval	104-354 300  300	$2.0 \times 10^{-11} \exp(107/T)$ $6.9 \times 10^{-11}$  $3.5 \times 10^{-37} \text{ cm}^6 \text{molecule}^{-2} \text{s}^{-1}$ (a) Derived from data in Kajimoto and Cvetanovic (1976a) and value of $k(\theta(^1\text{D}) + \text{N}_2)$ this survey	$\pm 0.1$   (a)
2,13	$\theta(^1\text{D}_2) + \text{N}_2\theta \rightarrow \text{N}_2 + \theta_2$ (a) $\rightarrow 2\text{N}\theta$ (b) †Davidson, et al (1977) Heidner, Husain (1973) †Cvetanovic (1975) review	204-359 300 300	$1.1 \times 10^{-10} (k_a + k_b)$ $2.2 \times 10^{-10} (k_a + k_b)$ $k_a/k_b = 1$	0.1
2,17	$\theta(^1\text{D}_2) + \text{NH}_3 \rightarrow \text{NH}_2 + \text{H}\theta$ †Davidson, et al (1977) Fletcher, Husain (1976a)	204-354 300	$2.5 \times 10^{-10}$ $6.3 \times 10^{-10}$	$\pm 0.1$

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of $\log k$
2,21	$\phi(^1\text{D}_2) + \text{H}_2 \rightarrow \text{H}\phi + \text{H}$ *Davidson, et al (1977) Heidner, Husain (1973)	204-352 300	$9.9 \times 10^{-11}$ $2.7 \times 10^{-10}$	
2,22	$\phi(^1\text{D}_2) + \text{H}_2\phi \rightarrow 2\text{H}\phi$ *Streit, et al (1976) Heidner, et al (1973)	253-353 300	$2.3 \times 10^{-10}$ $3.0 \times 10^{-10}$	$\pm 0.1$
2,23	$\phi(^1\text{D}_2) + \text{H}_2\phi_2 \rightarrow \text{H}\phi + \text{H}\phi_2$ Fletcher, Husain (1976a)	300	$5.2 \times 10^{-10}$	
2,39	$\phi(^1\text{D}_2) + \text{HCl} \rightarrow \text{products}$ *Davidson, et al (1977)	199-379	$1.4 \times 10^{-10}$	$\pm 0.1$
2,45	$\phi(^1\text{D}_2) + \text{C}\phi \rightarrow \text{C}\phi + \phi(^3\text{P})$ *This survey Heidner, et al (1973)	300 300	$3 \times 10^{-11}$ $7.3 \times 10^{-11}$	$\pm 0.3$ (a)
2,46	$\phi(^1\text{D}_2) + \text{C}\phi_2 \rightarrow \text{C}\phi_2 + \phi(^3\text{P})$ *Streit, et al (1976)		(a) $0.41 \times k$ of Heidner, et al; scaled to match other selected $\phi(^1\text{D})$ rates	
2,56	Fletcher, Husain (1976b) $\phi(^1\text{D}_2) + \text{CH}_4 \rightarrow \text{CH}_3 + \text{H}\phi$ (a) $\rightarrow \text{CH}_2\phi + \text{H}_2$ (b)	139-200 200-354 300	$1.2 \times 10^{-10}$ $6.8 \times 10^{-11} \exp(117/T)$ $1.7 \times 10^{-10}$	$\pm 0.1$ $\pm 0.1$
2,58	*Davidson, et al (1977) Heidner, Husain (1973) †Cvetanovic (1975) review $\phi(^1\text{D}_2) + \text{C}_2\text{H}_6 \rightarrow \text{products}$	198-357 300 300	$1.4 \times 10^{-10} (k_a + k_b)$ $3.1 \times 10^{-10} (k_a + k_b)$ $k_a/k_b = 10$	
	*This survey Fletcher, Husain (1976a)	300 300	$3 \times 10^{-10}$ $7.3 \times 10^{-10}$	$\pm 0.2$ (a)
2,61	$\phi(^1\text{D}_2) + \text{CF}_2\text{Cl}_2 \rightarrow \text{products}$ *NASA (1977) eval Fletcher, Husain (1976b)	300 300	(a) $0.41 \times k$ of Fletcher and Husain; scaled to match other selected $\phi(^1\text{D})$ rates	
2,62	$\phi(^1\text{D}_2) + \text{CFCl}_3 \rightarrow \text{products}$ *NASA (1977) eval Fletcher, Husain (1976b)	300 300	$2 \times 10^{-10}$ $4.8 \times 10^{-10}$	$\pm 0.2$ (a)
			(a) $0.41 \times k$ of Fletcher and Husain; scaled to match other selected $\phi(^1\text{D})$ rates	
3,1	$\phi(^1\text{S}) + \phi(^3\text{P}) \rightarrow ?$ Slanger, Black (1976a)	300 300	$2.3 \times 10^{-10}$ $5.5 \times 10^{-10}$	$\pm 0.2$ (a)
3,4	$\phi(^1\text{S}) + \phi_2 \rightarrow ?$	200-365 200-377	(a) $0.41 \times k$ of Fletcher and Husain; scaled to match other selected $\phi(^1\text{D})$ rates $5 \times 10^{-11} \exp(-305/T)$ $4.3 \times 10^{-12} \exp(-850/T)$	$\pm 0.15$ a

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of Log k
3,7	$\text{O}(^1\text{S}) + \text{O}_3 \rightarrow ?$	300	$5.8 \times 10^{-10}$	$\pm 0.07$ a
3,9	$\text{O}(^1\text{S}) + \text{NO} \rightarrow ?$	200-291	$3.2 \times 10^{-11} (\text{T})^{0.5}$	$\pm 0.05$ a
3,10	$\text{O}(^1\text{S}) + \text{NO}_2 \rightarrow ?$	300	$5 \times 10^{-10}$	$\pm 0.2$ a
3,12	$\text{O}(^1\text{S}) + \text{N}_2 \rightarrow ?$	200-380	$< 5 \times 10^{-17}$	a
3,13	$\text{O}(^1\text{S}) + \text{N}_2\text{O} \rightarrow ?$			
3,17	Slanger, Black (1976b) $\text{O}(^1\text{S}) + \text{NH}_3 \rightarrow ?$	200-368 300	$3.8 \times 10^{-11} \exp(-420/\text{T})$ $5 \times 10^{-10}$	$\pm 0.2$ a
3,22	$\text{O}(^1\text{S}) + \text{H}_2\text{O} \rightarrow ?$			
3,46	Bingham, et al (1976) $\text{O}(^1\text{S}) + \text{CO}_2 \rightarrow ?$	300 200-450	$1.3 \times 10^{-10}$ $3.1 \times 10^{-11} \exp(-1320/\text{T})$	$\pm 0.15$ a
3,56	$\text{O}(^1\text{S}) + \text{CH}_4 \rightarrow ?$	300	$2 \times 10^{-14}$	$\pm 0.4$ a
4,hv	$\text{O}_2 + \text{h}\nu \rightarrow \text{O}(^3\text{P}) + \text{O}(^3\text{P})$			
4,hv	Hampson, et al (1973a) review $\text{O}_2 + \text{h}\nu \rightarrow \text{O}(^3\text{P}) + \text{O}(^1\text{D})$		$\phi = 1$ $175 < \lambda < 200 \text{ nm}$	
4,hv	Hampson, et al (1973a) review $\text{O}_2 + \text{h}\nu \rightarrow 2 \text{ oxygen atoms}$		$\phi = 1$ $133 < \lambda < 175 \text{ nm}$	
4,hv	Hampson, et al (1973a) review $\text{O}_2 + \text{h}\nu$		$\phi = 1$ $106 < \lambda < 200 \text{ nm}$	
4,8	$\text{O}_2 + \text{N} \rightarrow \text{NO} + \text{O}$		Recommended values of absorption cross section $135 < \lambda < 243 \text{ nm}$	
4,9,9	$\text{O}_2 + \text{NO} + \text{NO} \rightarrow \text{NO}_2 + \text{NO}_2$ *Baulch, et al (1973) review Stedman, Niki (1973)	273-660 300	See reverse reaction $-\text{d}[\text{NO}]/\text{dt} = \text{d}[\text{NO}_2]/\text{dt} = 2k_1[\text{NO}]^2[\text{O}_2]$ $3.3 \times 10^{-39} \exp(530/\text{T}) \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ $2.0 \times 10^{-38}$	$\pm 0.2$ $\pm 0.1$
4,9,10	$\text{O}_2 + \text{NO} + \text{NO}_2 \rightarrow \text{NO}_2 + \text{NO}_3$		See reverse reaction	
4,9	$\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{O}$		See reverse reaction	
4,9M	$\text{O}_2 + \text{NO} + \text{M} \rightarrow \text{NO}_3 + \text{M}$		No recommendation	
4,10	Baulch, et al (1973) review $\text{O}_2 + \text{NO}_2 \rightarrow \text{NO} + \text{O}_3$		See reverse reaction	
4,11	$\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{O}_3$		See reverse reaction	
4,12	$\text{O}_2 + \text{N}_2 \rightarrow \text{N}_2\text{O} + \text{O}$			
	*Baulch, et al (1973) review	1200-2000	$1.0 \times 10^{-10} \exp(-55.2 \times 10^3/\text{T})$ (a) $k_f = k_r K_{\text{eq}}$ See reverse reaction	$\pm 0.4$ (a)
4,18	$\text{O}_2 + \text{H} \rightarrow \text{HO} + \text{O}$			
4,18M	$\text{O}_2 + \text{H} + \text{M} \rightarrow \text{HO}_2 + \text{M}$ (f)			
20,M	$\text{HO}_2 + \text{M} \rightarrow \text{O}_2 + \text{H} + \text{M}$ (r)			
	†This Survey			
	$k_f = 6.7 \times 10^{-33} \exp(290/\text{T}) \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$	203-404		$\pm 0.7$ (a)
	M = Ar or He, $k(300) = 1.8 \times 10^{-32}$			
	Rel. M efficiencies: Ar(1.0), He(1.0), N <sub>2</sub> (3.1), O <sub>2</sub> (3.1), H <sub>2</sub> O(25)			

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k
(a) This evaluation is based on the 300 K data reviewed by Baulch, et al (1972) and the recent studies by Hikida, et al (1971), Kurylo (1972) and Wong and Davis (1974).				
	Baulch, et al (1972) eval.	300-2000	$k_f = 4.1 \times 10^{-33} \exp(500/T)$ $M = \text{Ar}$ $\pm 0.2$ Rel. $M$ eff.: $\text{Ar}(1.0)$ , $\text{He}(1.0)$ , $\text{N}_2(1.3)$ , $\text{O}_2(1.3)$ , $\text{H}_2\text{O}(21)$ $k_r = k_f/K_{eq} = 3.5 \times 10^{-9} \exp(-23000/T)$ $M = \text{Ar}$ $\pm 0.2$ $k_f = 2.35 \times 10^{-32}$ $M = \text{Ar}$ $1.64 \times 10^{-32}$ $M = \text{Ar}$ $0.75 \times 10^{-32}$ $M = \text{He}$ Rel. $M$ efficiencies: $\text{He}(1.0)$ , $\text{Ar}(0.8)$ $1.4(\pm 0.14) \times 10^{-23} \exp(+700(\pm 50)/T)$ , $M = \text{Ar}$ Rel. $M$ eff.: at 297K: $\text{Ar}(1.0)$ , $\text{He}(0.97)$ , $\text{H}_2(1.28)$ .	
	Bishop, Dorfman (1970)	300		
	Hikida, Eyre, Dorfman (1971)	300		
	Ahumada, Michael, Osborne (1972)	300		
	Allen, Moortgat (1973)	115-300		
	Kurylo (1972)	203-404	$6.7 \times 10^{-33} \exp(235/T)$ Rel. $M$ eff.: $\text{Ar}(1.0)$ , $\text{He}(1.0)$ , $\text{N}_2(3.4)$	
	Wong, Davis (1974)	220-360	$6.8 \times 10^{-33} \exp(340/T)$ Rel. $M$ efficiencies: $\text{Ar}(1.0)$ , $\text{He}(0.93)$ , $\text{N}_2(2.8)$ , $\text{H}_2(3.0)$ , $\text{CH}_4(21.5)$	
	Westenberg, deHaas (1972a)	300	$1.9 \times 10^{-32}$ $M = \text{Ar or He}$	
	Slack (1977)	980-1176	$(9.1 \pm 1.6) \times 10^{-33}$ $M = \text{N}_2$	(a)
		964-1075	$(6.1 \pm 1.1) \times 10^{-23}$ $M = \text{Ar}$	(b)
		200-2000	$1.85 \times 10^{-28} T^{-1.42}$ $M = \text{N}_2$	
		200-2200	$5.8 \times 10^{-30} T^{-1}$ $M = \text{Ar}$	
4.21	$\text{O}_2 + \text{H}_2 \rightarrow \text{H} + \text{H}_2\text{O}$		(a) reanalysis of literature	
4.21	$\text{O}_2 + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$		(b) recommendation based on this work	
4.22	Baulch, et al (1972) review $\text{O}_2 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}_2 + \text{H}$		and data from literature	
4.23	Baulch, et al (1972) review $\text{O}_2 + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}$		see reverse reaction	
4.24	Baulch, et al (1972) review $\text{O}_2 + \text{HNO} \rightarrow \text{NO} + \text{H}_2\text{O}$		no recommendation	
4.27	Demerjian, et al (1974) review $\text{O}_2 + \text{SO} \rightarrow \text{SO}_2 + \text{O}$	300	no recommendation	estimated
4.31	$\text{O}_2 + \text{HS} \rightarrow \text{SO} + \text{H}_2\text{O}$	295	no recommendation	
4.35M	Cupitt, Glass (1974) $\text{O}_2 + \text{Cl} + \text{M} \rightarrow \text{ClO} + \text{M}$ (f)		$< 2.1 \times 10^{-20}$ , $F/R > 5000K$	
37.M	$\text{ClO} + \text{M} \rightarrow \text{Cl} + \text{O}_2 + \text{M}$ (r)		see reverse reaction	
	† NASA (1977) eval	200-300	$< 10^{-13}$ $k_r = 5.8 \times 10^{-9} \exp(-3580/T)$ (a) $k_r = k_f/K_{eq}$	(+2, -1) (a)

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k
4,46a	†Nicholas, Norrish (1968)	293	$k_f = 1.7 \times 10^{-33} \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$	
	Clyne and Coxon (1968)	300	$k_f = < 5.5 \times 10^{-33}$	
4,47	Stedman (1968)	200-300	$k_f = 5.5 \times 10^{-34}$ (b) As quoted by Clyne and Coxon (1968).	(b)
	$\phi_2 + \text{CN} \rightarrow \text{NC}\phi + \phi$	275-398	$5.3 \times 10^{-11} \exp(-500 \pm 170/T)$	
	Albers, et al (1975)	297	$k/k(\phi + \text{CH}\phi) = 2.74 \pm 0.21 \times 10^{-2}$	
4,49	Peeters, Mahnen (1973)	300	yielding $k = 5.7 \pm 1.2 \times 10^{-12}$	estimated
	$\phi_2 + \text{CH}_3 \rightarrow \text{CH}_2\phi + \text{H}\phi$	1400-1800	$1.7 \times 10^{-13}$ $5 \times 10^{-11}$	
	Washida, Bayes (1976)	259-341	$2.9 \times 10^{-13} \exp(-940/T)$	
	Basco, et al (1972)	295	$3 \times 10^{-16}$	estimated (a)
4,49M	$\phi_2 + \text{CH}_3(^1\text{M}) \rightarrow \text{CH}_3\phi_2(^1\text{M})$		a. Based on negative result and sensitivity limit. Other measurements at higher T suggest an appreciable activation energy.	
	Laufer, Bass (1975)	298	$10^{12} \frac{x}{k} \quad \frac{P(\text{N}_2)/\text{torr}}{50}$ 0.45 0.7 1.00 1.2 1.7 5.0 x 10 <sup>-13</sup> 1.9 x 10 <sup>-31</sup> cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> $\eta = \text{N}_2$	(a)
	Washida, Bayes (1976)	300	2.2 x 10 <sup>-12</sup> 5.1 x 10 <sup>-13</sup> 2.6 x 10 <sup>-31</sup> cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> $\eta = \text{N}_2$	(b) (b) (c)
	Hochanadel, et al (1977)	295	1.8 x 10 <sup>-12</sup> 6 x 10 <sup>-31</sup> cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> $\eta = \text{C}_3\text{H}_8$ preliminary	(b) (c)
	Basco, et al (1972)	295	(a) Values are based on $k(\text{CH}_3 + \text{CH}_3) = 9.5 \times 10^{-11}$ , given in Bass, Laufer (1973). (b) 2nd order high pressure limit. (c) 3rd order low pressure limit. see $\text{CH}_3\phi + \phi_2$	(b) (c)
4,50	$\phi_2 + \text{CH}_3\phi \rightarrow \dots$			
5,M	$\phi_2(^1\Delta) + \text{M} \rightarrow \phi_2 + \text{M}$	285-322	$2.2 \times 10^{-18} (T/300)^{0.8}$ $\eta = \phi_2$	$\pm 0.1$
	†Hampson, et al (1973) review	77	$1.1 \times 10^{-18}$ $\eta = \phi_2$	(a)
	Huestis, et al (1974)		(a) Liquid phase. When combined with gas phase data of Findlay and Snelling (1971a) (summarized in Hampson, et al (1973) $k = 2.2 \times 10^{-18} (T/300)^{0.5}$	



No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
	*Hampson, et al (1973) review	300	$< 2 \times 10^{-20}$ M = N <sub>2</sub>	
	Collins, et al (1973)	300	$1.4 \times 10^{-19}$ M = N <sub>2</sub>	±0.0e
	*Penzhorn, et al (1974)	300	$3.9 \times 10^{-20}$ M = S <sub>2</sub>	
	Penzhorn, et al (1975)	300	$2.1 \times 10^{-19}$ M = H <sub>2</sub> S	
		300	$k \times 10^{18}$ M	
			0.4 CF <sub>2</sub> Cl <sub>2</sub>	
			<0.08 CCl <sub>4</sub>	
			1.01 CH <sub>3</sub> Cl	
			0.87 CH <sub>2</sub> Cl <sub>2</sub>	
			0.92 CHCl <sub>3</sub>	
	Breckenridge, Miller (1972)	300	$< 2 \times 10^{-15}$ M = S <sub>2</sub>	(a)
	Fisher, McCarty (1966)	300	$< 3 \times 10^{-16}$ M = C <sub>2</sub>	(a)
			(a) total rate, quenching and reaction	
5,7	$\theta_2(^1\Delta) + \theta_3 \rightarrow 2\theta_2 + \theta$			
	Clark, Jones, Wayne (1970)	195-439	$6.6 \times 10^{-13}$ exp(-1560/T)	±0.24
	Findlay, Snelling (1971)	283-321	$4.5 \times 10^{-11}$ exp(-2830/T)	±0.11
	Becker, et al (1972)	296-360	$6.0 \times 10^{-11}$ exp(-2850/T)	±0.17
	Collins, et al (1973)	300	$4.4 \times 10^{-15}$	±0.11
	Schofield (1972) review	283-321	$4.5 \times 10^{-11}$ exp(-2830/T)	±0.11
	$\theta_2(^1\Delta) + N \rightarrow N\theta + \theta$			probably
5,8	Schmidt, Schiff (1973)	300	$k < k(N + \theta_2 \rightarrow N\theta + \theta)$	
	Westenberg, et al (1970)	195-300	$k < k(N + \theta_2 \rightarrow N\theta + \theta)$	
	Clark, Wayne (1970)	195-431	$k = 2 \times 10^{-14}$ exp(-600/T)	(a)
			(a) probably refers to physical deactivation, not chemical reaction; see above refs	
5,9	$\theta_2(^1\Delta) + N\theta \rightarrow \theta_2 + N\theta(v > 0)$			
	*Becker, et al (1971)	300	$4.5 \times 10^{-17}$	±0.15
	Yaron, et al (1976)	300	$2.5 \times 10^{-17}$	±0.1
	Giachardi, et al (1976)	293	$(4.5 \pm 1) \times 10^{-17}$	
	Øgrýzlo, Thrush (1973)	300	N $\theta(v = 4)$ observed	
	$\theta_2(^1\Delta) + H \rightarrow$ products			
5,18	Schmidt, Schiff (1973)	300	$(2.5 \pm 0.5) \times 10^{-14}$	(a)
			(a) expt could not distinguish between chemical rxn and physical quenching	
5,27	Westenberg, et al (1970)	300	rxn to give H $\theta + \theta$ as products not observed	
	$\theta_2(^1\Delta) + S\theta \rightarrow \theta_2 + S\theta(^1\Delta)$			
6,M	Breckenridge, Miller (1972)	300	$3.5 \pm 0.36 \times 10^{-13}$	
	$\theta_2(^1\Sigma) + M \rightarrow \theta_2 + M$			
	*Hampson, et al (1973) review	300	$1.5 \times 10^{-16}$ M = $\theta_2$	±0.12
			$2.0 \times 10^{-15}$ M = N <sub>2</sub>	±0.1
			$4 \times 10^{-12}$ M = H <sub>2</sub> $\theta$	±0.18



No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$		Notes and Reliability of log k
			$\sigma$	$\sigma^2$	
7, hv	$\sigma_3 + hv \rightarrow \sigma(^3P) + \sigma_2(^3\Sigma_g^-)$ *Hampson, et al (1973) review Johnston (1973)		$\sigma = 1, 450 < \lambda < 750 \text{ nm} = \text{Chappuis bands}$ $\sigma = 0, 250 < \lambda < 350 \text{ nm}$ $k = 3.39 \times 10^{-14} \text{ s}^{-1} \text{ (Daylight)}$ (450 < $\lambda$ < 750 nm = Chappuis bands)		
7, hv	$\sigma_3 + hv \rightarrow \sigma(^3P) + \sigma_2(^1\Delta \text{ or } ^1\Sigma)$ *This survey		$\sigma = 0, \lambda < 303 \text{ nm}$ Total quantum yield ( $\sigma^3P + \sigma^1D$ ) equals unity for 303 < $\lambda$ < 350 nm		
7, hv	$\sigma_3 + hv \rightarrow \sigma(^1D) + \sigma_2(^1\Delta)$ *Lin, DeMore (1973)				
7, hv					
7, hv					
7, M	Hampson, et al (1973) review $\sigma_3 + hv \rightarrow \sigma(^1D) + \sigma_2(^1\Sigma_g^+)$ *Hampson, et al (1973) review $\sigma_3 + M \rightarrow \sigma + \sigma_2 + M$ $\sigma_3 + N \rightarrow N\sigma + \sigma_2$ *NASA (1977) eval				
7, 8					
7, 9	Baulch, et al (1973) review $\sigma_3 + N\sigma \rightarrow N\sigma_2 + \sigma_2 (f)$ $\sigma_2 + N\sigma_2 \rightarrow N\sigma + \sigma_3 (r)$ *NASA (1977) eval	200-300	$2 \times 10^{-11} \exp(-1070/T)$ (a) Accepts room temp. rec. of Baulch "A factor" chosen; $P_{act}$ derived		$\pm 0.3 \text{ at } 230K$
4, 10		300	$5.7 \times 10^{-13}$		$\pm 0.2$
7, 9		200-300			
4, 10					
7, 9	Birks, et al (1976) Hampson, et al (1973) review Stedman, Niki (1973) Baulch, et al (1973) review	203-361 198-330 298 200-350 200-350 298 300 290	$k_f = 2.1 \times 10^{-12} \exp(-1450/T)$ (a) based on results in Birks et al (1976). Lower "A factor" derived from reconsideration of primary data $k_f = 2.34 \pm 0.23 \times 10^{-12} \exp(-1450 \pm 50/T)$ $k_f = 9 \times 10^{-13} \exp(-1200/T) \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}$ $k_f = 1.73 \pm 0.1 \times 10^{-14}$ $k_f = 1.5 \times 10^{-12} \exp(-1330/T)$ $k_f = k_f/K_{eq} = 2.8 \times 10^{-12} \exp(-25400/T)$ $k_f = 1.41 \times 10^{-14}$ $k_f = 1.81 \pm 0.13 \times 10^{-14}$ $k_f = 1.70 \times 10^{-14}$		$\pm 0.15 (a)$ $\pm 0.11$ $\pm 0.2$ $\pm 0.2$ $\pm 0.2$
7, 9	Chormley, et al (1973)				
4, 10	Bemand, et al (1974)				
7, 9	Becker, Schurath, Seitz (1974)				

7.9	$\sigma_3^* + N\sigma \rightarrow N\sigma_2^* (^2B_{1,2}) + \sigma_2$ (1) $\rightarrow N\sigma_2^* (^2A_1) + \sigma_2$ (2) $\rightarrow \sigma_3^* + N\sigma$ (3)	153-373 158-437 138-410	see discussion see discussion $k_1 = 1.0 \times 10^{-12} \exp(-1450/T)$ $k_2 = 3.8 \times 10^{-13} \exp(-520/T)$ $k_3 = 1.1 \times 10^{-13}$ at 333 K and at 143 K with minimum value of $0.62 \times 10^{-13}$ at approx. 230K
7.10 4.11	$\sigma_3^* + N\sigma_2 \rightarrow N\sigma_3^* + \sigma_2$ (f) $\sigma_2^* + N\sigma_3 \rightarrow \sigma_3^* + N\sigma_2$ (r) +NASA (1977) eval	220-340 260-343 231-298 259-362 286-302 300 299 298 298 289	<u>Discussion</u> Measured quantity in all studies is $(k_1 + k_2 + k_3)$ . Values of this quantity measured by Kurylo et al and by Hui, Cool are in good agreement; values reported by Bar-Ziv, Moy and Gordon are systematically higher below 300K. Hui and Cool derived values as a function of temperature for $k_1$ , $k_2$ , and $k_3$ given above from an analysis of the temperature dependent data for $(k_1 + k_2 + k_3)$ reported by the three groups, the temperature dependence of the enhancement factor for rxn channel (1) reported by Moy, Bar-Ziv and Gordon (1977), their own temperature dependent data for the ratio of the enhancement factors for rxn channels (1) and (2) and the rate constant for channels (1) and (2) for thermal ozone reported by Clough and Thrush (1967)
	Davis, Prusaczyk, Dwyer, Kim (1974) Graham, Johnston (1974) Hule, Herron (1974a) Baulch, et al (1973) review Wu, Morris, Niki (1973) Ghormley, et al (1973) Stedman, Niki (1973) Becker, Schurath, Seitz (1974)		$k_f = 1.2 \times 10^{-13} \exp(-2450/T)$ $k_f = 9.76 \pm 0.54 \times 10^{-14} \exp(-2427 \pm 140/T)$ $k_f = 1.34 \pm 0.11 \times 10^{-13} \exp(-2466 \pm 30/T)$ $k_f = 1.57 \pm 0.41 \times 10^{-13} \exp(-2509 \pm 76/T)$ $k_f = 9.8 \times 10^{-12} \exp(-3500/T)$ $k_f = 7 \times 10^{-34}$ based on $k_f$ $k_f = 4.4 \times 10^{-17}$ $k_f = 3.2 \times 10^{-17}$ $k_f = 6.5 \pm 0.8 \times 10^{-17}$ $k_f = 3.24 \times 10^{-17}$ (a) Derived by combining results from the three 1974 temperature dependent studies (b) Based on Johnston, Yost (1949) (c) Revision, based on later experiments, of value reported by Stedman and Niki (1973)

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k
7,18	$\text{O}_3 + \text{H} \rightarrow \text{HO} + \text{O}_2$ *Clyne, Monkhous (1977)	298-638	$1.0 \pm 0.2 \times 10^{-10} \exp(-516 \pm 50/T)$ (a) NASA (1977) evaluation selected preliminary value reported by these authors, $k = 1.2 \times 10^{-10} \exp(-550/T)$ with $\Delta \log k$ increased to $\pm 0.3$ at 230K.	$\pm 0.2$ (a)
	Lee, et al (1978) Phillips, Schiff (1962)	219-360 300	$1.3 \pm 0.3 \times 10^{-10} \exp(-449 \pm 58/T)$ $2.6 \pm 0.5 \times 10^{-11}$ (b) Quoted by Hampson, et al (1973) review and Baulch, et al (1976) review	(h)
7,19	$\text{O}_3 + \text{HO} \rightarrow \text{HO}_2 + \text{O}_2$ +*NASA (1977) eval	200-300	$1.5 \times 10^{-12} \exp(-1000/T)$ (a) *Adjusted from recommendation in Hampson et al (1973) review because of error in derivation of $\text{O}_3$ conc. from absorption meas.	$\pm 0.3$ (a)
	Hampson, et al (1973) review Anderson, Kaufman (1973) Baulch, et al (1976) review DeMore (1973) DeMore (1975)	220-450 220-450 300 300 271-233	$1.6 \times 10^{-12} \exp(-1000/T)$ $1.3 \times 10^{-12} \exp(-956/T)$ $6.5 \times 10^{-14}$ $8 \times 10^{-14}$ $k/k(\text{OH} + \text{O}) = 16.8 \exp(-1230/T)$ at 700 torr $\text{CO}_2$	$\pm 0.3$ $\pm 0.7$
7,19	Davis (1976) Kurylo (1973) $\text{O}_3 + \text{HO}(\text{v}_1 > 0) \rightarrow \text{products}$ Coltharp, Worley, Potter (1971)	300 298 300	$7.5 \pm 0.3 \times 10^{-14}$ $6.5 \times 10^{-14}$ $y_1(\text{HO})$	$\pm 0.06$
	Streit, Johnston (1976)		$10^{12} \times k(300 \text{ K})$ CWP SI	
		2 3 4 5 6 7 8 9	1.9 $\pm$ 1.1 2.4 $\pm$ 0.9 2.8 $\pm$ 0.8 3.4 $\pm$ 0.7 5.3 $\pm$ 0.6 6.5 $\pm$ 0.5 6.7 $\pm$ 0.5 7.7 $\pm$ 0.7	3.7 $\pm$ 0.1 4.5 $\pm$ 0.1 7.1 $\pm$ 0.2 8.5 $\pm$ 0.2 8.9 $\pm$ 0.2 11 $\pm$ 0.4
7,20	$\text{O}_3 + \text{HO}_2 \rightarrow \text{HO} + 2\text{O}_2$ +*NASA (1977) eval. Simonaitis, Heicklen (1973b) DeMore, Tschuikow-Roux (1974) Lloyd (1974) review Baulch, et al (1976) review	200-300 225-298 273-232 200-500 300	$7.3 \times 10^{-14} \exp(-1275/T)$ $k/(k_{\text{ref}})^{0.5} = 1.9 \times 10^{-8} \exp(-1000/T)$ $k/(k_{\text{ref}})^{0.5} = 1.1 \times 10^{-7} \exp(-1550 \pm 50/T)$ $1.7 \times 10^{-13} \exp(-1400/T)$ $1.5 \times 10^{-15}$ (a) $k_{\text{ref}} = k(\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2)$ Preferred value averages temp. dependence of these studies and is based on $k_{\text{ref}}$ value given in this table.	$\pm 0.2$ (a) (a) $\pm 0.3$ $\pm 0.2$

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
7,27	$\phi_3 + S\phi \rightarrow \phi_2 + S\phi_2$ Schofield (1973) review	223-303	$2.5 \times 10^{-12} \exp(-1050/T)$ no recommendation	$\pm 0.5$
7,28	Baulch et al (1976) review $\phi_3 + S\phi_2 \rightarrow S\phi_3 + \phi_2$			
7,32	Daubendiek, Calvert (1974) Davis, Prusaczyk, Dwyer, Kim (1974) $\phi_3 + H_2S \rightarrow$ products	300 300	$k < 8 \times 10^{-24}$ $k < 2 \times 10^{-22}$	
7,35	Glavas, Tohy (1975) Becker, Inocencio, Schurath (1975) $\phi_3 + Cl \rightarrow Cl\phi + \phi_2$	298-343 300	$7 \times 10^{-14} \exp(-3400/T)$ $< 2 \times 10^{-20}$	$\pm 0.4$
7,35Br	+Watson (1977) review Clyne, Nip (1976) Kurylo, Braun (1976) Watson, et al (1976) Zahniser, et al (1976) $\phi_3 + Br \rightarrow Br\phi + \phi_2$	205-298 221-629 213-298 220-350 210-360	$2.7 \times 10^{-11} \exp(-257/T)$ $5.18 \times 10^{-11} \exp(-418/T)$ $2.72 \times 10^{-11} \exp(-298/T)$ $3.08 \times 10^{-11} \exp(-250/T)$ $2.17 \times 10^{-11} \exp(-171/T)$	$\pm 0.12$ at 230K
7,36	+Leu, DeMore (1977) $\phi_3 + Cl\phi \rightarrow \phi Cl\phi + \phi_2$ (a) $\rightarrow Cl\phi\phi + \phi_2$ (b) +NASA (1977) eval	224-422 200-300	$3.34 \times 10^{-11} \exp(-978/T)$ $k_a = 1 \times 10^{-12} \exp(-4000/T)$ $k_b = 1 \times 10^{-12} \exp(-4000/T)$ $< 5 \times 10^{-15}$	$\pm 0.2$ at 230K $\pm 0.6, -2.0$ at 230K (a)
7,36Br	Watson (1977) review	300	(a) Based on unpublished 300K results of Lin and DeMore. Branching ratio unknown - assumed equal to unity.	
7,45	$\phi_3 + Br\phi \rightarrow$ products +Clyne, Cruse (1970) $\phi_3 + C\phi \rightarrow C\phi_2 + \phi_2$	293	$k < 1 \times 10^{-14}$	upper limit only
7,48	Arlin, Warneck (1972) $\phi_3 + CH_2\phi \rightarrow$ products	296	$< 4 \times 10^{-25}$	
7,49	Braslavsky, Heicklen (1976) $\phi_3 + CH_3 \rightarrow CH_3\phi + \phi_2$ (a) $\rightarrow CH_2\phi + H\phi_2$ (b) Simonalitis, Heicklen (1975)	300 221-298	$< 2 \times 10^{-24}$ $(k_a + k_b)/k_{ref} = 12 \exp(-525/T)$ (a) $k_{ref}$ is 2nd order high pressure limit for $CH_3 + \phi_2 (+M) \rightarrow CH_3\phi_2 (+M)$	$\pm 0.3$ upper limit (a)
7,51	$\phi_3 + CH_3\phi_2 \rightarrow$ products	300	$< 2.4 \times 10^{-17}$	
7,54	Simonalitis, Heicklen (1975) $\phi_3 + CH_3\phi\phi \rightarrow$	298-325	$6.8 \times 10^{-13} \exp(-5315/T)$	
7,56	Hastie, et al (1976) $\phi_3 + CH_4 \rightarrow$ products Dillemath, et al (1960)	310-340	$2.7 \times 10^{-13} \exp(-7700/T)$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
7,57	$\text{C}_3 + \text{C}_2\text{H}_4 \rightarrow \text{products}$ *Herron, Huie (1974) Demerjian, et al (1974) review DeMore (1969) Stedman, et al (1973) Davis (1974) Becker, Schurath, Seitz (1974) Japar, Wu, Niki (1974) Toby, et al (1976) $\text{C}_3 + \text{C}_3\text{H}_6 \rightarrow \text{products}$ *Herron, Huie (1974) Demerjian, et al (1974) review DeMore (1969) Stedman, et al (1973) Becker, Schurath, Seitz (1974) Japar, Wu, Niki (1974)	235-362 300 178-233 300 300 280-360 298 303	$9.0 \times 10^{-15} \exp(-2560/T)$ $2.7 \times 10^{-18}$ $3.2 \times 10^{-15} \exp(-2400/T)$ $1.55 \pm 0.15 \times 10^{-18}$ $1.6 \pm 0.2 \times 10^{-18}$ $1.2 \times 10^{-14} \exp(-2490 \pm 100/T)$ $1.9 \pm 0.1 \times 10^{-18}$ $1.7 \pm 0.1 \times 10^{-18}$	$\pm 0.1$
7,59	$\text{C}_3 + \text{allene} \rightarrow \text{products}$ Toby, Toby (1975)	275-362 300 183, 153, 300 300 280-360 298	$6.1 \times 10^{-15} \exp(-1900/T)$ $1.0 \times 10^{-17}$ $1.6 \times 10^{-15} \exp(-1600/T)$ $1.25 \pm 0.1 \times 10^{-17}$ $1.1 \times 10^{-14} \exp(-1970 \pm 100/T)$ $1.30 \times 10^{-17}$ (a) Includes 300 K point of Hanst et al (1958).	$\pm 0.1$ (a)
7,59	$\text{C}_3 + 1\text{-butene} \rightarrow \text{products}$ Huie, Herron (1975) Japar, Wu, Niki (1974) $\text{C}_3 + \text{cis-2-butene} \rightarrow \text{products}$ Huie, Herron (1975) Japar, Wu, Niki (1974) $\text{C}_3 + \text{trans-2-butene} \rightarrow \text{products}$ Huie, Herron (1975) Japar, Wu, Niki (1974) $\text{C}_3 + 1,3\text{-butadiene} \rightarrow \text{products}$ Toby, Toby (1975) Becker, Schurath, Seitz (1974) $\text{C}_3 + \text{cis-C}_2\text{Cl}_2\text{H}_2 \rightarrow \text{products}$ Blume et al (1976) $\text{C}_3 + \text{trans-C}_2\text{Cl}_2\text{H}_2 \rightarrow \text{products}$ Blume et al (1976) $\text{N} + \text{N} + \text{M} \rightarrow \text{N}_2 + \text{M}$ *Baulch, et al (1973) review	225-363 298 225-363 298 225-363 298 273-343 280-360 296 296 100-600	$2.9 \pm 0.2 \times 10^{-15} \exp(-1686 \pm 20/T)$ $1.23 \times 10^{-17}$ $3.1 \pm 0.7 \times 10^{-15} \exp(-956 \pm 54/T)$ $1.61 \times 10^{-16}$ $6.0 \pm 1.0 \times 10^{-15} \exp(-1051 \pm 43/T)$ $2.60 \times 10^{-16}$ $1 \times 10^{-13} \exp(-2900/T)$ $5.4 \times 10^{-14} \exp(-2680/T)$ $3.7 \times 10^{-20}$ $2.5 \times 10^{-19}$ $8.3 \times 10^{-34} \exp(+500/T) \text{cm}^6 \text{molecule}^{-2} \text{s}^{-1}$ $\text{M} = \text{N}_2$ where $-d[\text{N}]/dt = 2k[\text{N}]^2[\text{M}]$ $7.6 \times 10^{-32} \text{T}^{-1/2} \text{M} = \text{N}_2$	$\pm 0.7$ (a) $\pm 0.5$ $\pm 0.2$ (200-600K) $< 0.2$ (T < 200K)
7,59	Taylor (1975) review	2000-10000		



No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of $\log k$
8,9 1,12	$\text{N} + \text{N}\theta \rightarrow \text{N}_2 + \theta \text{ (f)}$ $\theta + \text{N}_2 \rightarrow \text{N} + \text{N}\theta \text{ (r)}$ +Clyne, McDermid (1975) Baulch, et al (1973) review	298-670 300-5000 2000-5000	$3.0 \times 10^{-32} \text{ T}^{-1/2}$ $\text{M} = \theta_2, \theta, \text{N}\theta$ $6.5 \times 10^{-27} \text{ T}^{-3/2}$ $\text{M} = \text{N}$ $k_f = 8.2 \times 10^{-11} \exp(-410/T)$ $k_f = 2.7 \times 10^{-11}$ $k_r = 1.3 \times 10^{-10} \exp(-38000/T)$ (a) Uncertainty increases to $\pm 0.3$ for $\text{T} > 2000$ . $k_f$ based on 300 K data and $k_r(\text{T} > 2000)$ .	$\pm 0.2$ at 230K $\pm 0.1$ (a) $\pm 0.7$
8,10	Taylor (1975) review $\text{N} + \text{N}\theta_2 \rightarrow \text{N}_2\theta + \theta$ +NASA (1977) eval. Clyne, McDermid (1975)	2000-10000 200-300 298	$k_f = 2.7 \times 10^{-11}$ $2 \times 10^{-11} \exp(-800/T)$ $1.4 \times 10^{-12}$ (a) Accepts room temp. result of Clyne + McDermid "A factor" chosen; Fact derived (b) Believed to be sole reaction channel	$\pm 0.2$ at 230K (a,b)
8,19	$\text{N} + \text{H}\theta \rightarrow \text{N}\theta + \text{H}$ +Baulch, et al (1973) review	300	$5.3 \times 10^{-11}$ (a) Based on $k/k(\theta + \text{H}\theta \rightarrow \theta_2 + \text{H}) = 1.4$	$\pm 0.3$ (a)
8,27	$\text{N} + \text{S}\theta \rightarrow \text{products}$ Baulch, et al (1976) review		no recommendation	
8,29	$\text{N} + \text{S}\theta_3 \rightarrow \text{products}$ Baulch, et al (1976) review		no recommendation	
8,37	$\text{N} + \theta \text{Cl}\theta \rightarrow \text{N}\theta + \text{Cl}\theta$ Watson (1977) review	298	$k < 6 \times 10^{-13}$	preliminary value
9, hv	$\text{N}\theta + \text{h}\nu$ Hampson, et al (1973a) review			
9, M	+Bethke (1959) $\text{N}\theta + \text{M} \rightarrow \text{N} + \theta + \text{M}$ Baulch, et al (1973) review	4200-6700	Recommended values of oscillator strengths from which absorption cross sections can be derived are given for $\beta$ , $\gamma$ , and $\epsilon$ bands. Recommended values of absorption cross section $106 < \lambda < 135 \text{ nm}$ . No recommended quantum yield values. Oscillator strength for $\delta$ bands, confirmed by Mandelman and Carrington (1974)	
9,9	$\text{N}\theta + \text{N}\theta \rightarrow \text{N} + \text{N}\theta_2$ Baulch, et al (1973) review		Insufficient data for a reliable recommendation. Use, with caution: $6.6 \times 10^{-4} \text{ T}^{-1.5} \exp(-75.5 \times 10^3/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ( $\text{M} = \text{Ar}, \theta_2, \text{N}_2$ ) $k(\text{M} = \text{N}\theta, \text{N}, \theta)/k(\text{Ar}) \sim 1:8$	
9,9	$\text{N}\theta + \text{N}\theta \rightarrow \text{N}_2\theta + \theta$		Endothermic. Unimportant compared to $\text{N}\theta + \text{N}\theta \rightarrow \text{N}_2\theta + \theta$ see reverse reaction	



No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
9,9,4	N $\theta$ + N $\theta$ + $\theta_2$ $\rightarrow$ N $\theta_2$ + N $\theta_2$		see $\theta_2$ + N $\theta$ + N $\theta$ $\rightarrow$ N $\theta_2$ + N $\theta_2$	
9,10,22	N $\theta$ + N $\theta_2$ + H $\theta_2$ $\rightarrow$ 2HN $\theta_2$ (f) 2HN $\theta_2$ $\rightarrow$ N $\theta$ + N $\theta_2$ + H $\theta_2$ (r) *Chan, et al (1976)	296	$k_f = 6.0 \times 10^{-38}$ cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> $k_r = 9.5 \times 10^{-19}$ cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> Reviewed earlier work, probably heterogeneous	
9,11	Hampson, et al (1973) review N $\theta$ + N $\theta_3$ $\rightarrow$ 2N $\theta_2$ Graham, Johnston (1978) Baulch, et al (1973) review Johnston (1966) review	300 300 300 300	(1.9 $\pm$ 0.4) $\times 10^{-11}$ $\sim 2 \times 10^{-11}$ 8.3 $\times 10^{-12}$ Temperature effect is probably zero or very small.	$\pm 0.7$ estimated
9,15	N $\theta$ + NH $\rightarrow$ products Hansen, et al (1976) Gordon, et al (1971) Mulvihill, Phillips (1975)	300 300 1500	4.7 $\times 10^{-11}$ 3.8 $\times 10^{-11}$ N $\theta_2$ + $\theta$ + H identified as products of major rxn channel	$\pm 0.1$
9,16	N $\theta$ + NH $\theta_2$ $\rightarrow$ N $\theta_2$ + H $\theta_2$ * *Hancock, et al (1975) Lesclaux, et al (1975)	298 300	2.1 $\times 10^{-11}$ 1.8 $\times 10^{-11}$ (a) $\gamma^{-1.25}$ dependence observed 300-500K	(a)
9,18M	Gehring, et al (1973) Gordon, et al (1971) N $\theta$ + H + M $\rightarrow$ HN $\theta$ + M *This survey	300 300	8 $\times 10^{-12}$ 2.7 $\times 10^{-11}$	$\pm 0.1$
9,19	Baulch, et al (1973) review	220-400 230-700 286-390 180-300 230-700 298-633	2.1 $\times 10^{-32}$ exp(300/T) M = H $\theta_2$ 1.5 $\times 10^{-32}$ exp(300/T) cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> M = H $\theta_2$ 2.5 $\times 10^{-32}$ exp(270/T) M = H $\theta_2$ 5.6( $\pm 0.6$ ) $\times 10^{-23}$ exp( $\pm 375(\pm 65)/T$ ), M = Ar 2 $\times 10^{-32}$ exp( $\pm 300/T$ ), M = H $\theta_2$ 5.2 $\times 10^{-12}$ exp( $-15.1 \times 10^3/T$ ) based on k = 5.8 $\times 10^{-10}$ exp( $-740/T$ ) for reverse reaction (a) corrected expression	$\pm 0.2$ (298K) (a) increasing to $\pm 0.3$ (623K)
9,19M	N $\theta$ + H $\theta$ (+M) $\rightarrow$ HN $\theta_2$ (+M) Hampson, et al (1973a) review	217 217 222 227 237 251 265 273-395	Elevation/km 15 20 25 30 35 40 45 2.2 $\times 10^{-32}$ exp( $\pm 1110/T$ ) cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> M=He $\pm 0.2$ at 300K (3rd order low pressure limit) k(T,M) 2.4 $\times 10^{-12}$ Abs. value of log k $\pm 0.5$ 1.5 $\times 10^{-12}$ Relative value of k 8.9 $\times 10^{-13}$ at different altitudes 4.8 $\times 10^{-13}$ reliable to $\pm 20\%$ 2.6 $\times 10^{-13}$ M = N $\theta_2$ 1.1 $\times 10^{-13}$ 5.9 $\times 10^{-14}$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k
9.20		300	$2 \times 10^{-12} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}$ (2d order high pressure limit) $5.8 \pm 1.2 \times 10^{-31} \times (295/T)^{2.4} \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ $M = \text{N}_2$ (3rd order low pressure limit) Relative efficiencies: $\text{N}_2(1.0)$ , $\text{Ar}(0.58)$ , $\text{He}(0.57)$	$\pm 0.7$
	Anderson, et al (1974)	295, 439		
	Howard, Evenson (1974)	296	$7.8 \pm 1.2 \times 10^{-31} \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ $M = \text{N}_2$ (3rd order low pressure limit) Relative efficiencies: $\text{N}_2(1.0)$ , $\text{Ar}(0.55)$ , $\text{He}(0.51)$	
	Cox (1974a)	294	$k/k(\text{H}\theta + \text{C}\theta) = 40 \pm 7$ $k = 1.2 \times 10^{-11} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}$ (a) 2nd order rate constant, $[M] = 1 \text{ atm } \text{N}_2 + \text{O}_2$ ; $k_{\text{ref}} = 3 \times 10^{-13}$ , this survey	(a)
	Harris, Wayne (1975)	300	$7 \pm 2 \times 10^{-31} \text{ cm}^6\text{molecule}^{-2}\text{s}^{-1}$ , $M = \text{Ar}$ $15 \pm 5 \times 10^{-31}$ , $M = \text{N}_2$ (3rd order low pressure limits)	
	Gordon, Mulac (1975)	435	$7.5 \pm 0.3 \times 10^{-12} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}$ (2nd order rate constant at 1 atm. $\text{H}_2\theta$ vapor)	
	Atkinson, Hansen, Pitts (1975a)	298	$4.94 \pm 0.5 \times 10^{-13}$ $M = 25 \text{ Torr } \text{N}_2$	(b)
	Cox, Derwent, Holt (1976)	298	(b) also data for $M = \text{Ar}$ at 25-655 torr $1.17 \times 10^{-11}$ $M = 1 \text{ atm } \text{N}_2 + \text{O}_2$	(c)
	Overend, et al (1976)	295	(c) relative to $k(\text{H}\theta + \text{H}_2) = 7 \times 10^{-15}$ $0.956 \pm 0.05 \times 10^{-12}$ $M = 25 \text{ torr } \text{N}_2$	
	Sie, et al (1976b)	298	$6.89 \pm 0.68 \times 10^{-12}$ $M = 770 \text{ torr } \text{N}_2$ $k/k_{\text{ref}} = 16.1$ at 95 torr and = 22 at 408 and 768 torr total pressure, mostly $\text{H}_2$ where ref rxn is $\text{H}\theta + \text{C}\theta \rightarrow \text{C}\theta_2 + \text{H}$	$\pm 0.4$ at 230K
9.20M	$\text{N}\theta + \text{H}\theta_2 \rightarrow \text{N}\theta_2 + \text{H}\theta$	296	$(8.1 \pm 1.5) \times 10^{-12}$	
	†Howard, Evenson (1977)	298-670	$2.0 \times 10^{-11} \exp(-1200/T)$	(a)
	Hack, et al (1975)	245-328	$k/(k_{\text{ref}})^{0.5} = 6.4 \times 10^{-6} \exp(-700/T)$	
	Simonaitis, Heicklen (1978)		(a) ref rxn: $2\text{H}\theta_2 \rightarrow \text{H}_2\theta_2 + \text{O}_2$	
	Cox, Derwent (1975)	296	$1.2 \times 10^{-12}$	$\pm 0.5$
9.21	Payne, Stief, Davis (1973)	300	$3 \times 10^{-13}$	$\pm 0.5$
	Glanzer, Troe (1975)	1350-1700	$7.5 \times 10^{-12}$	
	$\text{N}\theta + \text{H}\theta_2(+M) \rightarrow \text{H}\theta_3(+M)$			
	Cox, Derwent (1975)	296	$1.4 \times 10^{-13}$ at 1 atm $\text{N}_2 + \text{O}_2$	
9.21	Simonaitis, Heicklen (1976a)	296	$< 2 \times 10^{-15}$	
	$\text{N}\theta + \text{H}_2 \rightarrow \text{H}\theta + \text{H}$			
	Baulch, et al (1973) review	2000	$5.3 \times 10^{-18} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}$ (a) No data. Value based on reverse rate	$\pm 0.2$ (a)

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k
9,22	$\text{N}\delta + \text{H}_2\delta \rightarrow \text{HN}\delta + \text{H}\delta$ Baulch, et al (1973) review	2000	$4 \times 10^{-18}$ (a) No data. Value based on reverse rate. (corrected)	$\pm 0.2$ (a)
9,23	$\text{N}\delta + \text{H}_2\delta_2 \rightarrow \text{H}\delta + \text{HN}\delta_2$ *Hampson, et al (1973) review	300 500 300	$< 5 \times 10^{-20}$ $\sim 2 \times 10^{-20}$ $< 5 \times 10^{-20}$	
9,35M	Gray, et al (1972) $\text{N}\delta + \text{Cl} + \text{M} \rightarrow \text{ClN}\delta + \text{M}$ +*NASA (1977) eval	200-300	$1.7 \times 10^{-32} \exp(+530/T)$ $\text{M} = \text{N}_2$ (a) See Watson (1977) review	$\pm 0.6$ at 230K (a)
9,36	$\text{N}\delta + \text{Cl}\delta \rightarrow \text{N}\delta_2 + \text{Cl}$ +*NASA (1977) eval Watson (1977) review Zahniser, Kaufman (1977)	200-300 220-298 230-258	$1.0 \times 10^{-11} \exp(200 \pm 100/T)$ $8 \times 10^{-12} \exp(250/T)$ $k/k_{\text{ref}} = (0.52 \pm 0.05) \exp(373 \pm 23/T)$ (a) $k_{\text{ref}} = k(\text{Cl} + \delta_3)$	$\pm 0.3$ at 230K $\pm 0.1$ (a)
9,36Br	$\text{N}\delta + \text{Br}\delta \rightarrow \text{N}\delta_2 + \text{Br}$ +*NASA (1977) eval Clyne, Watson (1975) $\text{N}\delta + \delta\text{Cl}\delta \rightarrow \text{N}\delta_2 + \text{Cl}\delta$	200-300 298	$2.1 \times 10^{-11}$ $2.2 \times 10^{-11}$	$\pm 0.4$ at 230K $\pm 0.1$
9,37	+*NASA (1977) eval Bemand, Clyne, Watson (1973)	200-300 300	$2.5 \times 10^{-12} \exp(-600/T)$ $3.4 \times 10^{-13}$ (a) Based on room temp. value of Bemand, Clyne, Watson; temp dependence estimated	$\pm 0.6$ at 230K (a)
9,49M	$\text{N}\delta + \text{CH}_3 \rightarrow \text{M} \rightarrow \text{CH}_3\text{N}\delta \rightarrow \text{M}$ Laufer, Bass (1975)	298	$10^{11} \frac{x}{k}$ $\frac{P(\text{N}_2)}{50 \text{ torr}}$ .3 .45 1.1 100 700	(a) (b) (b)
9,50	$\text{N}\delta + \text{CH}_3\delta \rightarrow \dots$	298	$4 \times 10^{-12}$	
9,51	$\text{N}\delta + \text{CH}_3\delta_2 \rightarrow \text{CH}_3\delta_2\text{N}\delta$ (a) $\rightarrow \text{CH}_2\delta + \text{HN}\delta$ (b) $\rightarrow \text{CH}_3\delta + \text{N}\delta_2$ (c) +Demerjian, et al (1974) review Cox, et al (1976)	295 296 298	$1.7 \times 10^{-11}$ (a) Values are based on $k(\text{CH}_3 + \text{CH}_3) = 9.5 \times 10^{-11}$ given in Bass, Laufer (1973). (b) 2nd order high pressure limit. see $\text{CH}_3\delta + \text{N}\delta \rightarrow \dots$	estimate lower limit (a)
	$\text{N}\delta + \text{CH}_3\delta_2 \rightarrow \text{CH}_3\delta_2\text{N}\delta$ (a) $\rightarrow \text{CH}_2\delta + \text{HN}\delta$ (b) $\rightarrow \text{CH}_3\delta + \text{N}\delta_2$ (c) Pate, Finlayson, Pitts (1974) Simonaitis, Helcklen (1974)	296 298	$k_c = 3.3 \times 10^{-12} \exp(-500/T)$ $k_c \geq 1.2 \times 10^{-12}$ (a) based on value of $k(\text{CH}_3\delta_2 + \text{CH}_3\delta_2)$ Reaction proceeds exclusively through channel (c) $k_c/k = 0.80 \pm 0.15$ ( $k = k_a + k_b + k_c$ )	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k
10, hv	$\text{N}_2 + \text{h}\nu \rightarrow \text{N} + \text{N}$ *Bates (1974)		$\lambda/\text{nm}$ 295-358 398 400 405 410 $\phi(\text{P})$ 1.0 - 0.0008 ( $\lambda = 275$ ) 0.90 ± 0.05 0.76 ± 0.04 0.37 ± 0.02 0.14 ± 0.01 (a) Based on analysis of data in Jones and Bayes (1973) Extinction coefficient values tabulated for $\lambda = 185\text{-}410\text{nm}$ at 0.125nm intervals. Also gives values for $\text{N}_2\theta_4$ see reverse reaction	(a)
10, M	$\text{N}_2 + \text{M} \rightarrow \text{N} + \text{N} + \text{M}$		No recommendation	
10, 10	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ Baulch, et al (1973) review			
10, 10	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4 + \text{N}_2$ Baulch, et al (1973) review			
10, 10M	$\text{N}_2 + \text{N}_2 + \text{M} \rightarrow \text{N}_4 + \text{M}$ (f) $\text{N}_2\theta_4 + \text{M} \rightarrow \text{N}_2 + \text{N}_2 + \text{M}$ (r) Baulch, et al (1973) review	235-298	$3.3 \times 10^{-12} \exp(-13540/T)$ $k_1[\text{N}_2\theta_4]^2 = -(1/2)d[\text{N}_2]/dt$ increasing to 0.3 at 2000K	±0.15 (500-1000K)
10, 11	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ $\theta_2 + \text{N}_2 \rightarrow \text{N}_2 + \text{N}_2$ *Baulch, et al (1973) review	250-350	$k_f = 3.0 \times 10^{-35} \exp(1040/T)\text{cm}^6\text{molecule}^{-2}\text{s}^{-1}$ (a) corrected expression; $k_f = k_r k_{eq}$	M = $\text{N}_2$ ±0.15
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	250-350	$k_r = 4.2 \times 10^{-7} \exp(-5550/T)$	M = $\text{N}_2$ ±0.15
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	250-350	$k_r = 3.3 \times 10^{-7} \exp(-5540/T)$	M = $\text{N}_2$ ±0.15
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	300-850	$k_f = 2.3 \times 10^{-13} \exp(-1000/T)$	±0.4 (a)
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	300-500	$k_r = k_f/k_{eq} = 8 \times 10^{-41} \exp(400/T)\text{cm}^6\text{molecule}^{-2}\text{s}^{-1}$	±0.4
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	338-396	$k_f = 2.5 \times 10^{-14} \exp(-1230/T)$ (a) Based on $\text{N}_2\theta_5 + \text{M} \rightarrow \text{N}_2 + \text{N}_2 + \text{M}$ and $2\text{N}_2\theta_2 \rightarrow 2\text{N}_2 + \theta_2$	
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	217	Elevation/km k (T, M) $\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$ Log (M)	
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	217	15 1.9 x 10 <sup>-12</sup>	18.60
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	217	20 1.1 x 10 <sup>-12</sup>	18.27
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	222	25 6.6 x 10 <sup>-13</sup>	17.93
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	227	30 4.5 x 10 <sup>-13</sup>	17.58
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	237	35 2.7 x 10 <sup>-13</sup>	17.26
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	251	40 1.5 x 10 <sup>-13</sup>	16.92
10, 11M	$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_4$ This survey	265	45 7.1 x 10 <sup>-14</sup>	16.60



No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of log k
	Graham, Johnston (1978)	300	$k_f = 3.8 \times 10^{-12} \text{ cm}^3 \text{molecule}^{-1} \text{s}^{-1}$ (2d order high pressure limit)	$\pm 0.4$ (a)
		300-340	$k_r = 2.2 \times 10^{-5} \exp(-9700/T) \text{ cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	$\pm 0.3$ (a)
		273-300	$k_r = 5.7 \times 10^{14} \exp(-10600/T) \text{ s}^{-1}$ (limiting first order expression)	$\pm 0.4$ (a)
		298-329	$K_{eq} = 1.2 \times 10^{-27} \exp(-11180/T) \text{ cm}^3 \text{molecule}^{-1}$	
		273-300	$k_f(M) = 1.48 \times 10^{-13} \exp(-861/T) \text{ cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	(b)
			$k_r(M) = 1.24 \times 10^{14} \exp(-10317/T) \text{ s}^{-1}$	(c)
			(a) $k_f = K_{eq} k_r$ , $M = \text{N}_2, \text{O}_2, \text{NO}$	
			(b) 2d order rate const at 1 atm	
			(c) 1st order rate const at 1 atm	
		300	$k > k(\text{NO} + \text{NH}_2)$	
10,16	$\text{NO}_2 + \text{NH}_2 \rightarrow \text{products}$ Jayanty, et al (1975d)		$6.7 \times 10^{-12} \exp(-13900/T)$	
10,17	$\text{NO}_2 + \text{NH}_3 \rightarrow \text{NH}_2 + \text{HNO}_2$ Bedford, Thomas (1972)	615-660		
10,18	$\text{NO}_2 + \text{H} \rightarrow \text{HO} + \text{NO}$ Wagner, et al (1976a)			
	Clyne, Monkhous (1977)	243-461	$7.1 \times 10^{-10} \exp(-505 \pm 84/T)$	$\pm 0.1$
	Bemand, Clyne (1977)	298-653	$4.80 \times 10^{-10} \exp(-400 \pm 70/T)$	$\pm 0.1$
10,19M	$\text{NO}_2 + \text{HO} + \text{M} \rightarrow \text{HNO}_3 + \text{M}(\text{f})$	298	$1.13 \pm 0.22 \times 10^{-10}$	
26,M	$\text{HNO}_3 + \text{M} \rightarrow \text{HO} + \text{NO}_2 + \text{M}(\text{r})$ †NASA (1977) eval	200-350	$\log_{10}(k_f) = -A/T/(B + T) - 0.5 \log_{10}(T/280)$ $A = A_1 + A_2 Z + A_3 Z^2 + A_4 Z^3$ $B = B_1 + B_2 Z + B_3 Z^2$ $A_1 = 31.62273$ $A_2 = -0.258304$ $A_3 = -0.0889287$ $A_4 = 2.520173 \times 10^{-3}$ $B_1 = -327.372$ $B_2 = 44.5586$ $B_3 = -1.38092$	
			where $Z = \log_{10}[\text{N}_2]$ and is applicable only for the ranges 200<T/K<350 and $16.3 < \log_{10}[\text{N}_2]/\text{molecule} \cdot \text{cm}^{-3} < 15.5$ , with an estimated reliability in log k of $\pm 0.10$ (reliability analogous to log). Air is approximately 6 percent less efficient than nitrogen as a third body; i.e., $k$ for ( $M = \text{Air}$ ) = $0.94 k$ for $M = \text{N}_2$ For normal tropospheric conditions of 1 atm air and T = 300K, above expression yields value of $k_f = 1.1 \times 10^{-11}$	
	Anastasi, Smith (1976)	296	$k_f = 2.6 \times 10^{-30} M = \text{N}_2$ Rel. Efficiencies: $\text{N}_2(1.0)$ , $\text{He}(0.34)$ , $\text{Ar}(0.42)$ , $\text{O}_2(0.68)$ , $\text{SF}_6(2.5)$	
		220-550	$n = -2.6$ for temp dependence of form $T^n$ , $M = \text{N}_2$ values given for bimolecular rate constant over	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
			ranges T = 220-550K and [N <sub>2</sub> ] = 3 x 10 <sup>17</sup> to 1.6 x 10 <sup>19</sup> molecule cm <sup>-3</sup>	
	Baulch, et al (1973) review	273-400	k <sub>f</sub> = 3.6 x 10 <sup>-32</sup> exp(+1100/T)cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> M = He	±0.2
		800-1200	k <sub>r</sub> = 2.7 x 10 <sup>-9</sup> exp(-15400/T)cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> M = Ar	±0.4
		300	k <sub>f</sub> = 8 x 10 <sup>-12</sup> cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> (2d order high pressure limit)	±0.4
	Anderson, et al. (1974)	295-450	k <sub>f</sub> = 2.3 ± 0.5 x 10 <sup>-30</sup> x (295/T) <sup>2.5</sup> cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> M = N <sub>2</sub>	
			Relative efficiencies: N <sub>2</sub> (1.0), Ar(0.43), He(0.43)	
	Howard, Evenson (1974)	296	k <sub>f</sub> = 2.9 ± 0.4 x 10 <sup>-30</sup> M = N <sub>2</sub>	
	Gordon, Mulac (1975)	435	k <sub>f</sub> = 5.3 x 10 <sup>-12</sup> cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> (2nd order rate constant at 1 atm. H <sub>2</sub> O vapor)	
	Harris, Wayne (1975)	300	15 ± 5 x 10 <sup>-31</sup> cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> , M = Ar 26 ± 10 x 10 <sup>-31</sup> , M = N <sub>2</sub>	
	Atkinson, Perry, Pitts (1976)	298	k <sub>f</sub> = (1.0 ± 0.1) x 10 <sup>-30</sup> M = Ar Values given for bimolecular rate constant over pressure range 25-646 torr Ar	
10,20M	N <sub>2</sub> + H <sub>2</sub> O + M → H <sub>2</sub> O <sub>2</sub> + M †NASA (1977) eval	200-300	tentatively, use expression given for rxn 10,36M N <sub>2</sub> + Cl <sub>2</sub> + M → N <sub>2</sub> O <sub>2</sub> Cl <sub>2</sub> + M with twice the assigned uncertainty	
	Simonaitis, Heicklen (1978)	245 295	k[M]/k(H <sub>2</sub> O + N <sub>2</sub> ) = 0.61 (a) k[M]/k(H <sub>2</sub> O + N <sub>2</sub> ) = 0.036 (a) (a) M = 700 torr H <sub>2</sub> . Rxn to give H <sub>2</sub> NO + O <sub>2</sub> is negligible	(a) (a)
	Howard (1977)	300	(2.09 ± 0.52) x 10 <sup>-31</sup> M = N <sub>2</sub> Pel. eff: N <sub>2</sub> (1.0), He(0.48); O <sub>2</sub> (0.72); N <sub>2</sub> O <sub>2</sub> (3.2)	
	Cox, Derwent (1975)	298	k(H <sub>2</sub> O + N <sub>2</sub> → H <sub>2</sub> NO + O <sub>2</sub> ) < 3 x 10 <sup>-15</sup> k[M] = 1.2 x 10 <sup>-13</sup> for [M] = 1 atm product probably H <sub>2</sub> O <sub>2</sub> N <sub>2</sub> not H <sub>2</sub> NO + O <sub>2</sub> as assumed by authors	
10,28	N <sub>2</sub> + S <sub>2</sub> → S <sub>2</sub> + N <sub>2</sub>	300	k < 2 x 10 <sup>-24</sup>	
10,35M	Davis (1974) N <sub>2</sub> + Cl + M → N <sub>2</sub> O <sub>2</sub> Cl + M	298	7.2 x 10 <sup>-31</sup> cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup>	±0.6 at 230K
10,36M	†Clyne, White (1974) N <sub>2</sub> + Cl <sub>2</sub> + M → Cl <sub>2</sub> NO <sub>2</sub> + M †NASA (1977) eval	200-300	3.3 x 10 <sup>-23</sup> T <sup>-3.34</sup> 1 + 8.7 x 10 <sup>-9</sup> T <sup>-0.6</sup> [M] <sup>0.5</sup> (a) Expression developed by Zahniser, Chang, Kaufman (1977)	±0.6 at 230K (a)
	Birks, et al (1977)	250-356	(4.40 ± 0.66) x 10 <sup>-33</sup> exp(1087/T) M = N <sub>2</sub>	



No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Notes and Reliability of log k
10,49	Leu, Lin, DeMore (1977)	297	$9.57 \pm 0.28 \times 10^{-32}$	M = He
		258-417	$(3.69 \pm 0.24) \times 10^{-33} \exp(1150/T)$	M = N <sub>2</sub>
	Zahniser, Chang, Kaufman (1977)	248-417	$(2.66 \pm 0.35) \times 10^{-33} \exp(1140/T)$	M = He
		251-365	$(3.54 \pm 0.06) \times 10^{-33} \exp(950/T)$	M = He
		251-365	$5.53 \times 10^{-24} T^{-3.15}$	M = He
10,49M		297	$1.52 \times 10^{-31}$	M = N <sub>2</sub>
			(a) Two forms of temp dependence are given: $\exp(B/T)$ and $T^{-n}$	
	N <sub>2</sub> + CH <sub>3</sub> → CH <sub>3</sub> δ + N <sub>2</sub>			
	Glanzer, Troe (1973) review	300-1400	$3.3 \times 10^{-11}$	±0.25 (a)
			(a) Based on $k/k(\text{CH}_3 + \text{N}_2) = 3.3$ at room temperature and on shock wave pyrolysis of CH <sub>3</sub> N <sub>2</sub>	
10,49M	N <sub>2</sub> + CH <sub>3</sub> (→M) → CH <sub>3</sub> N <sub>2</sub> (→M)		$2.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	±0.1 (a)
	Glanzer, Troe (1973) review	295	(a) Based on high pressure limit rate ratio $k/k(\text{CH}_3 + \text{N}_2) = 1.7$	
10,49M	N <sub>2</sub> + CH <sub>3</sub> + M → CH <sub>3</sub> N <sub>2</sub> + M			
	Glanzer, Troe (1973) review	500-1400	$6.9 \times 10^{-31} \text{ cm}^6 \text{ molecule}^{-2} \text{ s}^{-1}$ , M = Ar	(a)
			(a) $k_f = k_r^{\text{eq}}$ see CH <sub>3</sub> δ + N <sub>2</sub> → . . .	
10,50 10,51	N <sub>2</sub> + CH <sub>3</sub> δ → . . .			
	N <sub>2</sub> + CH <sub>3</sub> δ → CH <sub>3</sub> δ <sub>2</sub> N <sub>2</sub> (a)			
	→ CH <sub>2</sub> δ + H <sub>2</sub> NN <sub>2</sub> (b) → CH <sub>3</sub> δ + N <sub>2</sub> (c)			
	*Heicklen (1973) review	298	$k_a/k = 0.75 \pm 0.05$ $k_b/k = 0.25 \pm 0.1$ $k_c/k < 0.1$	
11,11	N <sub>2</sub> + hν → N <sub>2</sub> + δ (1) → N <sub>2</sub> + δ <sub>2</sub> (2)			
	Graham, Johnston (1978)	300	table of absorption cross sections for wavelength region 400-700nm	(a)
			$J_1 = 0.099 \text{ s}^{-1}$ $J_2 = 0.04 \text{ s}^{-1}$	(b) (b)
			(a) This table also given in Molina's review (1977). Values supersede results in Johnston, Graham (1974)	
			(b) Specific photodissociation rates for troposphere with overhead sun. see reverse reaction	
11,M 11,11	N <sub>2</sub> + M → N <sub>2</sub> + δ + M			
	N <sub>2</sub> + N <sub>2</sub> → 2N <sub>2</sub> + δ <sub>2</sub>			
	Graham, Johnston (1978)	298-329	$8.5 \times 10^{-13} \exp(-2450/T)$	
	Baulch, et al (1973) review	293-309	$5 \times 10^{-12} \exp(-3000/T)$	±0.5 (a)
			(a) $-d[\text{N}_2]/dt = 2k[\text{N}_2]^2$ . Based on rate of δ <sub>3</sub> decomp. in presence of N <sub>2</sub> δ <sub>5</sub>	

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
11,22	N <sub>2</sub> O + H <sub>2</sub> O → HNO <sub>3</sub> + HO Baulch, et al (1973) review	300	2.3 x 10 <sup>-26</sup> (a) k <sub>f</sub> = k <sub>r</sub> K <sub>eq</sub>	±0.3 (a)
11,28	N <sub>2</sub> O + SO <sub>2</sub> → NO <sub>2</sub> + SO <sub>3</sub> Daubendiek, Calvert (1975) Davis (1976)	300 300	k < 7 x 10 <sup>-21</sup> k < 1 x 10 <sup>-21</sup>	preliminary
12,M	N <sub>2</sub> + M → N + N + M *Baulch, et al (1973) review	6000-15000	6.1 x 10 <sup>-3</sup> T <sup>-1.6</sup> exp(-113,200/T)cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> M = N <sub>2</sub>	±0.5
12,19	N <sub>2</sub> + HO → N <sub>2</sub> O + H *Baulch, et al (1973) review	700-2500	5.4 x 10 <sup>-12</sup> exp(-40.4 x 10 <sup>3</sup> /T) (a) k <sub>f</sub> = k <sub>r</sub> K <sub>eq</sub> (corrected expression)	±0.2 (a)
13,hv	N <sub>2</sub> O + hv → products Johnston, Selwyn (1975)	294	figures of absorption cross section vs λ for λ = 210-328nm. Negligible absorption for λ>260nm	
13,M	N <sub>2</sub> O + M → N <sub>2</sub> + O + M N <sub>2</sub> O + H → N <sub>2</sub> + HO Selwyn, et al (1977)	194-302	Absorption cross section values tabulated for λ = 173-240nm at 1 nm intervals for T = 194, 225, 243, 265 and 302K see reverse reaction	
13,18	N <sub>2</sub> O + M → N <sub>2</sub> + O + M N <sub>2</sub> O + H → N <sub>2</sub> + HO Albers, et al (1975)	718-1111 700-2500 773	(3.6 ± 1.2) x 10 <sup>-10</sup> exp(-8710 ± 350/T) 1.26 x 10 <sup>-10</sup> exp(-7600/T) 4.3 x 10 <sup>-15</sup>	±0.2 ±0.15
13,19	N <sub>2</sub> O + HO → products Chang, Kaufman (1977) Bierman, et al (1976) Atkinson, Perry, Pitts (1976)	480 298 298 443 440	< 4 x 10 <sup>-16</sup> 3.8 ± 1.2 x 10 <sup>-17</sup> < 2 x 10 <sup>-16</sup> < 2 x 10 <sup>-16</sup> < 2 x 10 <sup>-14</sup>	upper limit only
13,36	Gordon, Mulac (1975) N <sub>2</sub> O + ClO → products +NASA (1977) eval	200-300	k ≤ 1 x 10 <sup>-12</sup> exp(-4260/T) (a) "A factor" chosen. Fact fitted to upper limit at T = 587K reported in Watson's review (1977)	±2 at 230K (a)
13,45	N <sub>2</sub> O + CO → products Milks, Matula (1973)	1169-1655	3.5 x 10 <sup>-13</sup> exp(-8650/T)	
14,hv	N <sub>2</sub> O <sub>5</sub> + hv → . . . Molina (1977) review		table of absorption cross sections for wavelength range 206-380nm (a) Gives values for λ = 205-310nm from Graham, Johnston (1977) which supersede results in Johnston, Graham (1974). Also gives values for λ = 320-380nm from Jones, Wulf (1937)	(a)

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of $\log k$
Murphy (1969)				
Hampson, et al (1973a) review				
Daubendiek, Calvert (1974)				
14,M	$\text{N}_2\text{O}_5 (+M) \rightarrow \text{NO}_2 + \text{NO}_3 (+M)$ *This survey	217 217 222 227 237 251 265	$0.5 \times 10^{11} (-\text{N}_2\text{O}_5) = \beta(\theta) = 0.31 \lambda^{-1}$ $\lambda = 280 \text{ nm}$ Meas. by Holmes, Daniels (1934) are consistent Survey of photochemistry Figure giving molar extinction coefficient vs $\lambda$ . $250 < \lambda/\text{nm} < 350$ Elevation/km $k/\text{s}^{-1}$ 15 $5.0 \times 10^{-7}$ 20 $1.8 \times 10^{-7}$ 25 $3.0 \times 10^{-7}$ 30 $5.5 \times 10^{-7}$ 35 $1.9 \times 10^{-6}$ 40 $1.6 \times 10^{-5}$ 45 $4.4 \times 10^{-5}$ Extrapolated from data taken between 273 and 353 K. See reverse reaction	$\pm 0.5$
14,M	$\text{N}_2\text{O}_5 + M \rightarrow \text{NO}_2 + \text{NO}_3 + M$	300	$k < 1 \times 10^{-20}$	
14,22	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2\text{HNO}_3$	298	$< 1.3 \times 10^{-20}$	
Hampson, et al (1973) review				
Morris, Niki (1973)				
14,28	$\text{N}_2\text{O}_5 + \text{SO}_2 \rightarrow \text{products}$	300	$k < 4 \times 10^{-23}$	
Daubendiek, Calvert (1974)				
Davis (1974)				
16,18M	$\text{NH}_2 + \text{H} + M \rightarrow \text{NH}_3 + M$	300	$k < 8 \times 10^{-24}$	
Baulch, et al (1973) review				
16,19	$\text{NH}_2 + \text{H}_2 \rightarrow \text{NH}_3 + \text{H}$	2000-3000	$1.2 \times 10^{-33} \exp(11200/T) \text{ cm}^6 \text{ molecule}^{-2}\text{s}^{-1}$ , $M \rightarrow \text{Ar} \pm 0.3$ (a)	
16,21	$\text{NH}_2 + \text{H}_2 \rightarrow \text{NH}_3 + \text{H}$		(a) $k_f \rightarrow K_{\text{eq}} k_r$ See reverse reaction	
16,22	$\text{NH}_2 + \text{H}_2\text{O} \rightarrow \text{NH}_3 + \text{H}_2\text{O}$	800	$< 10^{-16}$ $k_f = K_{\text{eq}} k_r$	approximate
17,M	$\text{NH}_3 + M \rightarrow \text{NH}_2 + \text{H} + M$		no data, no recommendation	
Baulch, et al (1973) review				
17,18	$\text{NH}_3 + \text{H} \rightarrow \text{NH}_2 + \text{H}_2$	2000-3000	$k = 1.5 \times 10^{-8} \exp(-42400/T) (M = \text{Ar})$ (a) To be used when $P(M) < 4 \text{ atm}$ .	$\pm 0.7$ (a)
17,19	$\text{NH}_3 + \text{H}_2 \rightarrow \text{NH}_2 + \text{H}_2$	800	$< 10^{-16}$	approximate
Baulch, et al (1973) review				
*Smith, Zellner (1975)				
Perry, Atkinson, Pitts (1976a)				
Davis (1977)				
Cox, Derwent, Holt (1975)				
Hack, et al (1974)				
Stuhl (1973a)				
Kurylo (1973)				
Gordon, Mulac (1975)				
17,18	$\text{NH}_3 + \text{H} \rightarrow \text{NH}_2 + \text{H}_2$	228-472	$2.3 \times 10^{-12} \exp(-800/T)$	$\pm 0.1$
17,19	$\text{NH}_3 + \text{H}_2 \rightarrow \text{NH}_2 + \text{H}_2$	298-427	$2.93 \times 10^{-12} \exp(-850 \pm 150/T)$	preliminary
		300	$(1.4 \pm 0.1) \times 10^{-13}$	
		300	$(1.2 \pm 0.4) \times 10^{-13}$	
		298-669	$5.3 \pm 0.8 \times 10^{-12} \exp(-920/T)$	
		298	$1.5 \times 10^{-13}$	$\pm 0.1$
		298	$4.1 \times 10^{-14}$	$\pm 0.06$
		418	$4.2 \pm 0.5 \times 10^{-13}$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of $\log k$
17,36	$\text{NH}_3 + \text{ClO} \rightarrow \text{products}$ Walker (1972)	670	$k < 5 \times 10^{-16}$ (a) As quoted by Watson (1977) review.	(a)
17a,18	$\text{N}_2\text{H}_4 + \text{H} \rightarrow \text{H}_2 + \text{N}_2\text{H}_3$ Stief, Payne (1976)	228-400	$(9.87 \pm 1.17) \times 10^{-12} \exp(-1200 \pm 50/T)$	
18,18M	$\text{H} + \text{H} + \text{M} \rightarrow \text{H}_2 + \text{M} \text{ (f)}$			
21,M	$\text{H}_2 + \text{M} \rightarrow \text{H} + \text{H} + \text{M} \text{ (r)}$ Baulch, et al (1972) review	300 1700-5000	$k_f = 8.3 \times 10^{-23} \text{ cm}^6 \text{molecule}^{-2} \text{s}^{-1} \quad \text{M} = \text{H}_2$ $= 1.8 \times 10^{-30} \text{ T}^{-1} \quad \text{M} = \text{Ar}$ Rel. efficiencies: $\text{H}_2(1.0)$ , $\text{Ar}(0.25)$ $-d[\text{H}]/dt = 2k[\text{H}]^2[\text{M}]$ $k_r = 3.7 \times 10^{-10} \exp(-48300/T) \text{ cm}^3 \text{molecule}^{-1} \text{s}^{-1}$ $\text{M} = \text{Ar}$ see reverse reaction	$\pm 0.2$ $\pm 0.3$ $\pm 0.3$
18,19	$\text{H} + \text{HO} \rightarrow \text{H}_2 + \text{O}$			
18,19M	$\text{H} + \text{HO} + \text{M} \rightarrow \text{H}_2\text{O} + \text{M} \text{ (f)}$			
22,M	$\text{H}_2\text{O} + \text{M} \rightarrow \text{H} + \text{HO} + \text{M} \text{ (r)}$ *Baulch, et al (1972) review	1000-3000 2000-6000	$k_f = 6.1 \times 10^{-26} \text{ T}^{-2} \text{ cm}^6 \text{molecule}^{-2} \text{s}^{-1}, \text{M} = \text{N}_2$ $k_r = 5.8 \times 10^{-9} \exp(-52900/T) \text{ cm}^3 \text{molecule}^{-1} \text{s}^{-1}$ $\text{M} = \text{N}_2$ $k_f = 4.3 \times 10^{-25} \text{ T}^{-2.6} \quad \text{M} = \text{He}$ Rel eff: $\text{He}(1.0)$ , $\text{Ar}(1.5)$ , $\text{N}_2(3.2)$	$\pm 0.3$ $\pm 0.2$ $\pm 0.3$
18,20	Zellner, Erler, Field (1977)	230-300		
18,20	$\text{H} + \text{HO}_2 \rightarrow \text{HO} + \text{HO} \text{ (1f)}$			
19,19	$\text{HO} + \text{HO} \rightarrow \text{H} + \text{HO}_2 \text{ (1r)}$			
18,20	$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2 \text{ (2)}$			
18,20	$\text{H} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O} \text{ (3)}$ Baulch, et al (1972) review	290-800	$k_{1f} = 4.2 \times 10^{-10} \exp(-950/T)$ $k_{1r} = k_{1f}/K_{eq} = 2.0 \times 10^{-11} \exp(-20200/T)$ $k_2 = 4.2 \times 10^{-11} \exp(-750/T)$ $k_{2r} = k_{2f}/K_{eq} = 9.1 \times 10^{-11} \exp(-29100/T)$ $k_3 = \text{no recommendation}$ $k_{1f}$ and $k_2 = \text{same as Baulch, et al}$ $k_3 = 8.3 \times 10^{-11} \exp(-500/T)$ $k_{1f} = 8.3 \times 10^{-12}$ $k_2 = 1 \times 10^{-11}$ $k_3 = 6.7 \times 10^{-12}$	$\pm 0.3 \text{ (a)}$ $\pm 0.3$ $\pm 0.4$ $\pm 0.4$ $> \pm 0.7 \text{ (a)}$ $> \pm 0.5 \text{ (b)}$ $? \text{ (c)}$ $? \text{ (c)}$ $? \text{ (c)}$
	Lloyd (1974) review	300-1000		
	Moortgat, Allen (1973)	297		
	(a) Reaction 1 and rate ratios control values for reactions 2 and 3. (b) Temperature coefficient estimated. (c) Secondary reaction in $\text{H} + \text{O}_2 + \text{M}$ systems, fit of concentration vs. time plots.			

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>2</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
18,22	H + H <sub>2</sub> O → H <sub>2</sub> + HO Baulch, et al (1972) review	300-2500	1.5 x 10 <sup>-10</sup> exp(-10250/T)	±0.06 at 300K increasing to ±0.2 at high temp.
18,23	H + H <sub>2</sub> O <sub>2</sub> → H <sub>2</sub> + HO <sub>2</sub> (a) → HO + H <sub>2</sub> O (b) *Klemm, Payne, Stief (1975) Gorse, Volman (1974)	283-353 300	k <sub>a</sub> + k <sub>b</sub> = 5.2 ± 2.0 x 10 <sup>-12</sup> exp(-1400 ± 140/T) k <sub>a</sub> = 3.1 ± 0.8 x 10 <sup>-15</sup> k <sub>b</sub> = 5.7 ± 1.4 x 10 <sup>-15</sup>	
	Hampson, et al (1973)	300-800	k <sub>a</sub> = 2.8 x 10 <sup>-12</sup> exp(-1900/T) k <sub>b</sub> no recommendation (a) Accepts recommendations of Baulch, et al (1972). k <sub>b</sub> /k <sub>a</sub> = 1.3	(a) (a)
18,24	Meagher, Heicklen (1975) H + HNO → H <sub>2</sub> + NO Hampson, et al (1973) review Baulch, et al (1973) review	298 211-703 2000 300 2000	> 5 x 10 <sup>-14</sup> 7 x 10 <sup>-12</sup> 10 <sup>-13</sup> < k < 10 <sup>-12</sup> 8 x 10 <sup>-12</sup>	±0.3 ±0.3 ±0.2
18,25	H + HNO <sub>2</sub> → products Hampson, et al (1973) review Baulch, et al (1973) review		No data No recommendation	
18,26	H + HNO <sub>3</sub> → products Hampson, et al (1973) review Chapman, Wayne (1974) Baulch, et al (1973) review	300 300 300	< 1 x 10 <sup>-13</sup> < 2 x 10 <sup>-15</sup> < 10 <sup>-13</sup>	approximate upper limit
18,28M	H + SO <sub>2</sub> + M → SO <sub>3</sub> + M Baulch, et al (1976) review	1650-2120	1.4 x 10 <sup>-32</sup>	±0.2
18,31 21,26a	H + HS → H <sub>2</sub> + S (f) H <sub>2</sub> + S → H + HS (r) Baulch, et al (1976) review	298	k <sub>f</sub> = 2.5 x 10 <sup>-11</sup> k <sub>r</sub> = 2.2 x 10 <sup>-25</sup> (a) k <sub>r</sub> = k <sub>f</sub> /K <sub>eq</sub> k <sub>f</sub> = 2.5 ± 0.8 x 10 <sup>-11</sup>	±0.2 ±0.2 (a)
18,32	Cupitt, Glass (1974) H + H <sub>2</sub> S → H <sub>2</sub> + HS Kurylo, Peterson, Braun (1971)	295 190-464	1.29 x 10 <sup>-11</sup> exp(860/T) (a) Selected by Baulch, et al (1976) review	(a)
18,34c	H + COS → CO + HS Baulch, et al (1976) review	300	2.2 x 10 <sup>-14</sup>	±0.2
18,37	H + ClO → HO + Cl *Watson (1977) review	298	5.7 ± 1.2 x 10 <sup>-11</sup>	



No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
18,39	H + HCl → H <sub>2</sub> + Cl Ambidge, et al (1976a)	298-521	7.8 x 10 <sup>-12</sup> exp(-1600±84/T)	
18,42	H + N <sub>2</sub> O → HCl + NO Spencer, Glass (1975)	295	4.3 x 10 <sup>-14</sup>	
18,44	H + N <sub>2</sub> O → HCl + NO Wagner, et al (1976a)	255-461	7.6 x 10 <sup>-11</sup> exp(-457 ± 72/T)	
	H + Cl <sub>2</sub> → HCl + Cl *This survey	250-700	1.46 x 10 <sup>-10</sup> exp(-593/T)	±0.1 (a)
18,45M	H + CO + M → HCO + M Baulch, et al (1976) review	300-730	(a) Based on data in Remand, Clyne and Wagner, et al (1.41 ± 0.24) x 10 <sup>-10</sup> exp(-575 ± 65/T)	
18,46	H + CO <sub>2</sub> → HCO + CO Wagner, et al (1976)	252-458	(1.44 ± 0.28) x 10 <sup>-10</sup> exp(-600 ± 70/T)	
18,48	H + CH <sub>2</sub> O → H <sub>2</sub> + CH <sub>2</sub> Ambidge, et al (1976)	292-434	(7.6 ± 2.2) x 10 <sup>-11</sup> exp(-714 ± 100/T)	
18,53	H + CH <sub>3</sub> COOH → CH <sub>3</sub> O + H <sub>2</sub> O (a) Ridley, et al (1972) Westenberg, deHaas (1972b) H + CH <sub>3</sub> COOH → CH <sub>3</sub> O + H <sub>2</sub> O (b) → CH <sub>3</sub> O <sub>2</sub> + H <sub>2</sub> (c) → CH <sub>2</sub> COH + H <sub>2</sub> (c) Slemr, Warneck (1977)	298-773 297 297-652 250-358	2.0 x 10 <sup>-33</sup> exp(-850/T), M = H <sub>2</sub> see reverse reaction 5.4 x 10 <sup>-14</sup> 2.2 x 10 <sup>-11</sup> exp(-1890/T) k = (2.8 ± 0.9) x 10 <sup>-13</sup> exp(-930 ± 95/T) k <sub>a</sub> /k = 0.43 ± 0.07 k <sub>b</sub> /k = 0.52 ± 0.07 k <sub>c</sub> /k = 0.05	overall rate const ±0.12 ±0.04
18,54	H + CH <sub>3</sub> ONH → CH <sub>3</sub> OH + NO (a) → CH <sub>2</sub> ONH + H <sub>2</sub> (b) → CH <sub>3</sub> O + HNO (c) Moortgat, et al (1977)	223-398	k = (4.3 ± 0.9) x 10 <sup>-13</sup> exp(-950 ± 55/T) k <sub>a</sub> /k = 0.47 ± 0.05 (k <sub>b</sub> + k <sub>c</sub> )/k = 0.53 ± 0.05	overall rate const
18,64	H + CH <sub>3</sub> Cl → HCl + CH <sub>3</sub> Westenberg, deHaas (1975a)	500-800	6.2 x 10 <sup>-11</sup> exp(-4650/T)	
19,M	H <sub>2</sub> + M → H + H + M Baulch, et al (1972) review		no recommendation (E/R > 50000 K) see reverse reaction	
19,19	H <sub>2</sub> + H <sub>2</sub> → H + H <sub>2</sub> H <sub>2</sub> + H <sub>2</sub> → H <sub>2</sub> + H <sub>2</sub> Baulch, et al (1972) review		no recommendation	
19,19	H <sub>2</sub> + H <sub>2</sub> → H <sub>2</sub> + H <sub>2</sub> (f) H <sub>2</sub> + H <sub>2</sub> → H <sub>2</sub> + H <sub>2</sub> (r) *Baulch, et al (1972) review	300-2000 300-2000 1500-2000	k <sub>f</sub> = 1.0 x 10 <sup>-11</sup> exp(-550/T) k <sub>r</sub> = 1.1 x 10 <sup>-10</sup> exp(-9240/T) k <sub>f</sub> = 5.1 x 10 <sup>-11</sup> exp(-3500/T)	±0.2 ±0.2
1,22	H <sub>2</sub> + H <sub>2</sub> → H <sub>2</sub> + H <sub>2</sub> (r) *Baulch, et al (1972) review	300	k <sub>r</sub> = 2.3 x 10 <sup>-12</sup>	±0.06
	Rawlins, Gardiner (1974) Westenberg, deHaas (1973a)			



No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
19,19M 23,M	McKenzie, et al (1973)	298	k <sub>f</sub> = 2.1 ± 0.5 x 10 <sup>-12</sup>	
	Clyne, Down (1974)	300	k <sub>f</sub> = 1.4 ± 0.2 x 10 <sup>-12</sup>	
		300	k <sub>f</sub> = 1.7 ± 0.6 x 10 <sup>-12</sup>	(a)
	Trainor, von Rosenberg (1974)	300	k <sub>f</sub> = 2.1 ± 0.2 x 10 <sup>-12</sup>	
	Wilson (1972) review	300	k <sub>f</sub> = 2.57 x 10 <sup>-12</sup>	+0.1, -0.5
19,19M 23,M	Hθ + Hθ + N → H <sub>2</sub> θ <sub>2</sub> + M (f)		(a) Evaluation based on authors' work and other recent data	
	H <sub>2</sub> θ <sub>2</sub> + M → Hθ + Hθ + M (r)		-d[OH]/dt = 2k[OH] <sup>2</sup> [M]	
	+NASA (1977) eval	200-300	k <sub>f</sub> = 1.25 x 10 <sup>-32</sup> exp(900/T)	(a)
	Trainor, von Rosenberg (1974)	300	(a) Accepts room temp value of Trainor, von Rosenberg. E/R value chosen same as for comb. of θH with Nθ	
	Baulch, et al (1972) review	700-1500	k <sub>f</sub> = 2.5 ± 0.3 x 10 <sup>-31</sup> M = N <sub>2</sub> k <sub>f</sub> = 2.5 x 10 <sup>-33</sup> exp(+2550/T)cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> M = N <sub>2</sub>	±0.1 700<T<950K
19,20	Hθ + Hθ <sub>2</sub> → H <sub>2</sub> θ + θ <sub>2</sub>		k <sub>r</sub> = 2.0 x 10 <sup>-7</sup> exp(-22900/T)cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	±0.3 at 1500K
	+NASA (1977) eval	200-300	M = N <sub>2</sub> ; k <sub>f</sub> = k <sub>r</sub> K <sub>eq</sub>	
	Burrows, Harris, Thrush (1977)	293	3 x 10 <sup>-11</sup>	0.5 at 230K
		300-1000	5.1 x 10 <sup>-11</sup>	(a)
	Lloyd (1974) review	300	(a) Based on k(Hθ + H <sub>2</sub> θ <sub>2</sub> ) = 7.9 x 10 <sup>-13</sup>	
19,21	Hochanadel, et al (1972)	300	8.7 x 10 <sup>-11</sup> exp(-500/T)	±0.2
	DeMore, Tschuikow-Roux (1974)	300	2 x 10 <sup>-10</sup>	
		300	1.1 x 10 <sup>-10</sup>	±0.5 (a)
			(a) Adjusted value = based on reported ratio and values of k(θ <sub>3</sub> + Hθ) and k(Hθ <sub>2</sub> + Hθ <sub>2</sub> ) in this survey.	
	Hθ + H <sub>2</sub> → H <sub>2</sub> θ + H			
19,21	+Baulch, et al (1972) review	300-2500	3.6 x 10 <sup>-11</sup> exp(-2590/T) cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	±0.08 at 700K ±0.2 at high temp.
	Wilson (1972) review	300-2000	3.8 x 10 <sup>-11</sup> exp(-2600/T)	±0.3
	Stuhl, Niki (1972)	298	7.1 x 10 <sup>-15</sup>	±0.06
	Westenberg (1973a)	298	7.6 x 10 <sup>-15</sup>	±0.04
		352	1.8 x 10 <sup>-14</sup>	
		403	3.2 x 10 <sup>-14</sup>	
		518	1.4 x 10 <sup>-13</sup>	
		628	3.6 x 10 <sup>-13</sup>	
		745	6.6 x 10 <sup>-13</sup>	
	Smith, Zellner (1974a)	210-460	1.8 x 10 <sup>-11</sup> exp(-2330/T)	
	Gardiner, et al (1974)	1350-1600	8.7 x 10 <sup>-11</sup> exp(-3250/T)	
	Greiner (1969)	300-500	6.8 x 10 <sup>-12</sup> exp(-2020/T)	±0.15
	Atkinson, Hansen, Pitts (1975)	297-434	5.9 x 10 <sup>-12</sup> exp(-2008 ± 150/T)	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^2\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of $\log k$
19,21	Overend, et al (1975)	295	$(5.80 \pm 0.26) \times 10^{-15}$	
19,22	Trainor, von Rosenberg (1975)	300	$5.3 \times 10^{-15}$	
19,23	Vandooren, et al (1975)	600-1300	$1.2 \times 10^{-11} \exp(-2200/T)$	
	$\text{H}\theta + \text{D}_2 \rightarrow \text{HD}\theta + \text{D}$			
	Smith, Zellner (1974a)	210-460	$1.25 \times 10^{-11} \exp(-2550/T)$	
	$\text{H}\theta + \text{H}_2\theta \rightarrow \text{H}_2\theta_2 + \text{H}$		no recommendation	$\pm 0.3$ at 230K (a)
	Baulch, et al (1972) review			
	$\text{H}\theta + \text{H}_2\theta_2 \rightarrow \text{H}_2\theta + \text{H}\theta_2$			
	†NASA (1977) eval	200-300	$1 \times 10^{-11} \exp(-750/T)$	
	Hack, et al (1975)	298-670	$8.0 \times 10^{-12} \exp(-670/T)$	
	Greiner (1968)	300-458	$4.1 \times 10^{-13} T^{1/2} \exp(-600/T)$	
	Hampson (1973) quoting	300-800	$1.7 \times 10^{-11} \exp(-910/T)$	$\pm 0.2$
	Baulch, et al (1972) review			
	Gorse, Volman (1972)	300	$k/k(\text{H}\theta + \text{C}\theta) = 8.13$	
	Meagher, Heicklen (1974)	298	$k/k(\text{H}\theta + \text{C}\theta) = 4.1 \pm 0.6$	
19,24	$\text{H}\theta + \text{HN}\theta \rightarrow \text{H}_2\theta + \text{N}\theta$		(a) Based on results of Hack, et al (1975) and Greiner (1968)	
19,25	Hampson, et al (1973) review	1600-2100	$7 \times 10^{-11}$	$\pm 0.7$
	Baulch, et al (1973) review	2000	$6 \times 10^{-11}$	$\pm 0.2$
	$\text{H}\theta + \text{HN}\theta_2 \rightarrow \text{H}_2\theta + \text{N}\theta_2$			
	Cox, Derwent, Holt (1976)	296	$(6.6 \pm 0.3) \times 10^{-12}$	
			ref. rxn is $\text{H}\theta + \text{H}_2 \rightarrow \text{H}_2\theta + \text{H}$ with $k_{\text{ref}} = 7 \times 10^{-15}$	
19,26	Cox (1974a)	294	$k/k(\text{H}\theta + \text{C}\theta) = 15 \pm 1$ at 1 atm air	$\pm 0.1$ at 230K (a)
	$\text{H}\theta + \text{HN}\theta_3 \rightarrow \text{H}_2\theta + \text{N}\theta_3$			
	†Smith, Zellner (1975)	240-406	$8 \pm 2 \times 10^{-14}$	
	Margitan, et al (1975)	270-470	$8.9 \pm 1.3 \times 10^{-14}$	
	Hampson, et al (1973) review	300-650	$6 \times 10^{-13} \exp(-400/T)$	
	Johnston (1974) review	300-700	$(1.5 \text{ to } 2.0) \times 10^{-13}$	
	Baulch, et al (1975) review	300	$1.3 \times 10^{-13}$	
19,28M	$\text{H}\theta + \text{S}\theta_2 + \text{M} \rightarrow \text{HS}\theta_3 + \text{M}$		(a) Value recommended by authors for $T \leq 298\text{K}$ .	
	Davis (1976)	300	$10^{13} \frac{\text{K}}{\text{K}}$	(a)
			$0.87 \pm 0.06$	
		150	$1.6 \pm 0.1$	
		500	$2.7 \pm 0.2$	
			$10^{13} \frac{\text{K}}{\text{K}}$	
		50	$1.37 \pm 0.06$	
		150	$2.50 \pm 0.3$	
		500	$3.71 \pm 0.3$	
			$10^{13} \frac{\text{K}}{\text{K}}$	
		5	$0.08 \pm 0.08$	
		10	$1.43 \pm 0.14$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of log k
			$2.44 \pm 0.3$	
			20	
			760	
			(b) Extrapolated value.	
	Harris, Wayne (1975)	300	$4.5 \pm 1.5 \times 10^{-31} \text{ cm}^6 \text{molecule}^{-2} \text{s}^{-1}$ , $M = \text{Ar}$	
			$7.2 \pm 2.6 \times 10^{-31}$ , $M = \text{N}_2$	
	Cox (1974a)	294	$k/k(\text{H}\theta + \text{C}\theta) = 4 \pm 0.5$	(c)
			(c) 2nd order rate constant, $[M] = 1 \text{ atm. N}_2 + \theta_2$	
			see entry for $k(\text{H}\theta + \text{C}\theta)$	
	Gordon, Mulac (1975)	435	$1.8 \times 10^{-12} \text{ cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	
			(2d order rate constant at 1 atm. $\text{H}_2\theta$ vapor)	
	Castleman, Tang (1977)	297	$1.6 \times 10^{-31} \text{ cm}^6 \text{molecule}^{-2} \text{s}^{-1}$ , $M = \text{N}_2$	
			$k/k(\text{H}\theta + \text{C}\theta) = 4.3$	(d)
			(d) Measured ratio of 2d order rate constants at 1 atm $\text{N}_2$ .	
			Values for k given in paper assumed $k_{\text{ref}} = 1.5 \times 10^{-12}$	
			over entire pressure range. See entry for $k(\text{H}\theta + \text{C}\theta)$	
	Atkinson, Perry, Pitts (1976)	298	$10^{13} \frac{k}{k_{\text{ref}}}$	(e)
			1.35	
			2.16	
			3.10	
			4.38	
			5.87	
			6.55	
			(e) Effective 2nd order rate constant in $\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	
19,32	$\text{H}\theta + \text{H}_2\text{S} \rightarrow \text{H}_2\theta + \text{HS}$			
	Baulch, et al (1976) review	300-500	$1.05 \times 10^{-11} \exp(-200/T)$	$\pm 0.15$
	Perry, Atkinson, Pitts (1976a)	297-427	$(5.2 \pm 0.5) \times 10^{-12}$	
	Stuhl (1974)	298	$3.1 \pm 0.5 \times 10^{-12}$	
			see reverse reaction	
19,35	$\text{H}\theta + \text{Cl} \rightarrow \theta + \text{HCl}$			
19,39	$\text{H}\theta + \text{HCl} \rightarrow \text{H}_2\theta + \text{Cl}$			
	†Watson (1977) review	220-300	$3.0 \times 10^{-12} \exp(-425/T)$	$\pm 0.1$ at 230K
	Smith, Zellner (1974a)	210-460	$4.1 \times 10^{-12} \exp(-530/T)$	
	Zahniser, et al (1974)	224-460	$2.0 \pm 0.1 \times 10^{-12} \exp(-312 \pm 10/T)$	
	Takacs, Glass (1973)	295	$6.4 \pm 1.5 \times 10^{-13}$	$\pm 0.1$
	Davis (1974)	300	$6.5 \pm 0.4 \times 10^{-13}$	
19,39	$\text{H}\theta + \text{DCI} \rightarrow \text{HD}\theta + \text{Cl}$			
	Smith, Zellner (1974a)	210-460	$4.7 \times 10^{-12} \exp(-780/T)$	
19,39Br	$\text{H}\theta + \text{HBr} \rightarrow \text{H}_2\theta + \text{Br}$			
	†Takacs, Glass (1973)	300	$5.1 \times 10^{-12}$	$\pm 0.36$ at 230K
19,43a	$\text{H}\theta + \text{N}\theta_3\text{Cl} \rightarrow \text{products}$			
	†Zahniser, et al (1977)	246-387	$(1.19 \pm 0.10) \times 10^{-12} \exp(-333 \pm 22/T)$	$\pm 0.36$ at 230K
19,45	Ravishankara, et al (1977)	245	$3.7 \times 10^{-13}$	
18,46	$\text{H}\theta + \text{C}\theta \rightarrow \text{C}\theta_2 + \text{H}$ (f)			
	$\text{H} + \text{C}\theta_2 \rightarrow \text{H}\theta + \text{C}\theta$ (r)			
	†NASA (1977) eval	200-400	$k_f = 1.4 \times 10^{-13}$	low pressure value
				$\pm 0.1$

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of log k
*Baulch, et al (1976) review		250-2500	$\log k_f = -12.95 + 3.94 \times 10^{-4} \times T$ same as given in Baulch, Drysdale (1974) recommendation based on low pressure studies	$\pm 0.1$
		1000-3000	$k_r = k_f/K_{eq} = 2.5 \times 10^{-10} \exp(-13300/T)$	$\pm 0.1$
		300	$k_f = 3.0 \times 10^{-13}$ (a) Tentative rec. 1 atmosphere air have shown an apparent increase in k in the presence of $\text{SF}_6$ , $\text{H}_2$ , $\text{N}_2/\theta_2$ but not He or Ar.	$\pm 0.1$ (a)
			Biermann, et al (1978) have identified a combined effect of inert gas and $\theta_2$ . Trace impurities of $\theta_2$ have a significant effect and 1 torr is sufficient to produce the limiting rate constant in the presence of 1 atm of $\text{N}_2$ .	
Butler, et al (1977)		298	<u>Experiments bearing on the "pressure effect"</u> Mole fractions	
			$k_f/k_{ref}$	$\text{N}_2 - \text{C}_2 - \text{C}_2\theta$
			0.094	100
			0.10	0.49/0.33/0.15
			0.17	0.50/0.34/0.15
			0.15	0.73/0.17/0.08
			0.16	0.50/0.34/0.15
			0.18	0.73/0.17/0.07
				0.74/0.17/0.08
			Ref. rxn is $\text{H}\theta + \text{isobutane} \rightarrow \text{products}$ , with 6-28% correction for side rxn. Ratios calculated from reported data using authors' value for $k_{ref} = 1.59 \times 10^{-12}$ which was determined in the 100 torr expt. relative to $k(\text{H}\theta + \text{C}\theta) = 1.5 \times 10^{-13}$	
Chan, et al (1977)		298	$k_f/k_{ref}$	P/torr
			0.059	100 in "synthetic air"
Sie, Simonaitis, Heicklen (1976a)		217-298 298	0.127	700
			Ref. rxn is $\text{H}\theta + \text{isobutane} \rightarrow \text{products}$	
			$k_f/k_{ref}$	P/torr
			0.2exp(1700/T)	high pressure limit in $\text{H}_2$
			14	20 ( $\text{H}_2$ )
			21	83 ( $\text{H}_2$ )
			42	296 ( $\text{H}_2$ )
			49	702 ( $\text{H}_2$ )
			17	605 ( $\text{He}$ ) + 2 $\theta$ ( $\text{H}_2$ )
			33	550 ( $\text{SF}_6$ ) + 2 $\theta$ ( $\text{H}_2$ )
Cox, Derwent, Holt (1976)		296	49	605 ( $\text{SF}_6$ ) + 2 $\theta$ ( $\text{H}_2$ )
			Ref. rxn is $\text{H}\theta + \text{H}_2 \rightarrow \text{H}_2\theta + \text{H}$	
			$k_f/k_{ref}$	P/torr
Atkinson, Perry, Pitts (1976)		299	38.6	700 $\text{N}_2/\theta_2 = 2$
			Ref. rxn. is $\text{H}\theta + \text{H}_2 \rightarrow \text{H}_2\theta + \text{H}$	
			(1.54 $\pm$ 0.16) $\times 10^{-13}$ P = 25-654 torr Ar	

No.	Reaction/Reference * - Preferred Value † - NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$		Notes and Reliability of log k
			$10^{13} \frac{x}{k}$	$\frac{P(\text{SF}_6)}{\text{torr}}$	

19.48	Perry, Atkinson, Pitts (1977a)	299	1.53 1.93 2.40 3.09 3.42	25 76 208 403 603	
	Everend, Paraskevopoulos (1977)	296	(2.03 $\pm$ 0.08) $\times 10^{-13}$ at 50 torr He (3.24 $\pm$ 0.20) $\times 10^{-13}$ at 200, 350 torr SF <sub>6</sub>		
	Gordon, Mulac (1975)	298	1.50 $\times 10^{-13}$ at 710 torr Ar, 10 torr H <sub>2</sub> <sup>o</sup>		
	Trainor, von Rosenberg (1975)	300	Experiments either at low pressure or for which pressure effects were not studied.		
	Vandooren, et al (1975)	400-800	1.25 $\times 10^{-13}$ 1.33 $\times 10^{-13}$ 3.85 $\times 10^{-12}$ exp(-2850/T) 7.8 $\times 10^{-13}$		
	Blordi, et al (1975)	1350-1750	log k = -12.93 + 4.0 $\times 10^{-4}$ x T		$\pm 0.3$
	Steinert, Zellner (1975)	300-900	5.1 $\times 10^{-13}$ exp(-300/T)		$\pm 0.06$
	Wilson (1972) review	300-2000	1.35 $\times 10^{-13}$		$\pm 0.04$
	Stuhl, Niki (1972)	300	1.33 $\times 10^{-13}$		
	Westenberg, deHaas (1973a)	298	1.38 $\times 10^{-13}$		
		396	1.44 $\times 10^{-13}$		
		523	1.69 $\times 10^{-13}$		
		707	2.17 $\times 10^{-13}$		
		915	2.15 $\pm$ 0.15 $\times 10^{-13}$ exp(-80 $\pm$ 40/T)		$\pm 0.04$
	Davis, Fischer, Schlif (1974)	220-373	2.1 $\times 10^{-13}$ exp(-115/T)		$\pm 0.1$
	Greiner (1969)	300-500	1.45 $\times 10^{-13}$		(h)
	Smith, Zellner (1973)	300	(b) Data reported 210 < T < 460 K. Slight positive temperature dependence, possibly curved.		
			4.7 $\times 10^{-13}$		
		1600-1900	6.7 $\times 10^{-12}$ exp(-4000/T)		
		1500-2000	1.56 $\pm$ 0.2 $\times 10^{-13}$		
	Peeters, Mahnen (1973)	296	3 $\times 10^{-11}$ exp(-250/T)		$\pm 0.4$ at 230K (a)
	Gardiner, et al (1973)	300	1.4 $\times 10^{-11}$		$\pm 0.1$
	Howard, Evenson (1974)	300-1600	8 $\times 10^{-11}$		$\pm 1$
	H <sub>2</sub> + CH <sub>3</sub> <sup>o</sup> $\rightarrow$ H <sub>2</sub> <sup>o</sup> + CH <sub>3</sub> <sup>o</sup>	1400-1800	3.8 $\times 10^{-11}$		
	†NASA (1977) eval	200-300	(a) "A factor" chosen; E <sub>act</sub> fitted to room temp value of Morris, Niki		
19.52	H <sub>2</sub> + CH <sub>3</sub> <sup>o</sup> H $\rightarrow$ products				
19.54	Campbell, et al (1976)	292	9.5 $\times 10^{-13}$		
	H <sub>2</sub> + CH <sub>3</sub> NO <sub>2</sub> $\rightarrow$ products				
19.54	Campbell, Goodman (1975b)	292	9.2 $\times 10^{-13}$		
	H <sub>2</sub> + CH <sub>3</sub> ONO $\rightarrow$ products				
	Campbell, Goodman (1975b)	292	1.3 $\times 10^{-12}$		



No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
19,56	H <sub>2</sub> + CH <sub>4</sub> → CH <sub>3</sub> + H <sub>2</sub> θ			
	†Davis, Fischer, Schliff (1974)	240-373	2.36 ± 0.21 x 10 <sup>-12</sup> exp(-1710 ± 88/T)	±0.04
	Margitan, et al (1974)	290-440	3.83 x 10 <sup>-12</sup> exp(-1840 ± 20/T)	±0.06
	Wilson (1972) review	300-2000	4.7 x 10 <sup>-11</sup> exp(-2500/T)	±0.7
	Overend, et al (1975)	300	6.51 ± 0.26 x 10 <sup>-15</sup>	
	Peeters, Mahnen (1973)	1100-1900	5 x 10 <sup>-11</sup> exp(-3000/T)	
	Greiner (1970)	300-500	5.5 x 10 <sup>-12</sup> exp(-1900/T)	±0.1
	Gordon, Mulac (1975)	381	2.6 x 10 <sup>-14</sup> (1 atm H <sub>2</sub> θ vapor)	
		416	5.5 x 10 <sup>-14</sup> (1 atm H <sub>2</sub> θ vapor)	
		Zellner, Steinert (1976)	300-900	5.76 x 10 <sup>-21</sup> T <sup>3.08</sup> exp(-1010/T)
19,56a	Howard, Evenson (1976)	296	(9.5 ± 1.4) x 10 <sup>-15</sup>	
	Cox, Derwent, Holt (1976)	296	(7.3 ± 0.9) x 10 <sup>-15</sup>	
			ref rxn is H <sub>2</sub> θ + H <sub>2</sub> → H <sub>2</sub> θ + H with k <sub>ref</sub> = 7 x 10 <sup>-15</sup>	
	H <sub>2</sub> + C <sub>2</sub> H <sub>2</sub> → products			
	Smith, Zellner (1973)	210-460	2.0 x 10 <sup>-12</sup> exp(-250/T)	
	Pastrana, Carr (1974)	300	2.0 ± 0.6 x 10 <sup>-13</sup>	
	Davis, et al (1975)	300	1.65 ± 0.15 x 10 <sup>-13</sup>	
	H <sub>2</sub> + C <sub>2</sub> H <sub>4</sub> → products			
	Atkinson, Perry, Pitts (1977)	299-425	2.2 x 10 <sup>-12</sup> exp(385 ± 150/T)	(a)
			(a) High pressure values (225-660 torr Ar) Values also given for 25 and 75 torr pressure dependent values given over range 1 to 7 torr He 1.0 ± 0.2 x 10 <sup>-11</sup>	(b)
19,57	Howard (1976)	296		
	Overend, Paraskevopoulos (1977)	296		
			(b) Authors' suggested limiting high pressure value based on expts at 400 torr SF <sub>6</sub> and CF <sub>4</sub> and analysis of dependence of k on [H <sub>2</sub> θ] at low values of [H <sub>2</sub> θ]	
	Stuhl (1973c)	298	3 x 10 <sup>-12</sup>	±0.12
	Smith, Zellner (1973)	210-460	7.5 x 10 <sup>-12</sup> exp(-110/T)	
	Davis, et al (1975)	300	10 <sup>-12</sup> x k 2.24 2.78 3.63 4.06 4.72 5.33	P(He)/torr 3 5 10 20 100 300
		300	3.64 x 10 <sup>-12</sup> at 3 torr N <sub>2</sub>	
		300	1.8 x 10 <sup>-12</sup>	
		300	1.7 ± 0.5 x 10 <sup>-12</sup>	
		300-500	1.26 x 10 <sup>-12</sup> exp(454/T) at 100 torr He	
	381	6.2 x 10 <sup>-12</sup> (1 atm H <sub>2</sub> θ vapor)		
	416	7.3 x 10 <sup>-12</sup> (1 atm H <sub>2</sub> θ vapor)		

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^2\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of $\log k$
19,58	$\text{H}\theta + \text{C}_2\text{H}_6 \rightarrow \text{products}$ Overend, et al (1975) Greiner (1970)	300 300-500 296	$2.64 \pm 0.17 \times 10^{-13}$ $1.86 \times 10^{-11} \exp(-1230/T)$ $(2.9 \pm 0.6) \times 10^{-13}$	
19,59	$\text{H}\theta + \text{C}_3\text{H}_8 \rightarrow \text{products}$ Atkinson, Pitts (1975b) Stuhl (1973c) Morris, et al (1971) Bradley, et al (1973) Gorse, Volman (1974)	297-425 298 300 300 300	$4.1 \times 10^{-12} \exp(540 \pm 150/T)$ $1.45 \times 10^{-11}$ $1.7 \times 10^{-11}$ $5.0 \pm 1.7 \times 10^{-12}$ $k/k(\text{C}\theta + \text{H}\theta) = 89.3$ (low pressure) $k = 1.2 \times 10^{-11}$	$\pm 0.06$     (a)
19,60	$\text{H}\theta + n\text{-C}_4\text{H}_{10} \rightarrow \text{products}$ Stuhl (1973b) Perry, Atkinson, Pitts (1976b) Greiner (1970) Gorse, Volman (1974)	300 297-420 300-500 300	$(a) k(\text{C}\theta + \text{H}\theta) = 1.4 \times 10^{-13}$ , this survey $1.53 \pm 0.06 \times 10^{-11}$ $1.4 \times 10^{-11}$ (1 atm $\text{H}_2\theta$ vapor) $2.0 \times 10^{-11}$ (1 atm $\text{H}_2\theta$ vapor)  $2.35 \times 10^{-12}$ $1.76 \times 10^{-11} \exp(-560/T)$ $1.41 \times 10^{-11} \exp(-524/T)$ $k/k(\text{C}\theta + \text{H}\theta) = 19.4$ (low pressure) $k = 2.7 \times 10^{-12}$	           (a)
19,60	$\text{H}\theta + \text{isobutane} \rightarrow \text{products}$ Greiner (1970) Gorse, Volman (1974)	300-500 300	$(a) k(\text{C}\theta + \text{H}\theta) = 1.4 \times 10^{-13}$ , this survey  $8.7 \times 10^{-12} \exp(-387/T)$ $k/k(\text{H}\theta + \text{C}\theta) = 23.5$ (low pressure) $k = 3.3 \times 10^{-12}$	   (a)
19,60	$\text{H}\theta + \text{alkane} \rightarrow \text{H}_2\theta + \text{alkyl radical}$ Greiner (1970)	300	$(a) k(\text{C}\theta + \text{H}\theta) = 1.4 \times 10^{-13}$ , this survey $1.6 \times 10^{-12}$  (b) Determined in expt. at 100 torr relative to $k(\text{H}\theta + \text{C}\theta) = 1.5 \times 10^{-13}$	(b)
19,60a	$\text{H}\theta + \text{C}_6\text{H}_6 \rightarrow \text{products}$ Perry, Atkinson, Pitts (1977)	298 380-470 298	$k = [1.0 \exp(-820/T) N_p + 2.3 \exp(-430/T) N_s + 2.1 \exp(+95/T) N_t] \times 10^{-12}$ Where $N_p$ , $N_s$ , and $N_t$ are the number of primary secondary, and tertiary hydrogen atoms respectively. Do not use formula for $\text{CH}_4$ and $\text{C}_2\text{H}_6$ .  $(1.20 \pm 0.15) \times 10^{-12}$ $k_1 = 4 \times 10^{-11} \exp(-2000/T)$ $k_1/k = 0.05$	total rxn; $P = 100$ torr Ar (a) (b)
	Hansen, Atkinson, Pitts (1975)	298	(a) $k_1$ refers to abstraction rxn (b) Fraction of rxn proceeding by abstraction; expression for $k_1$ extrapolated to 298K  $(1.24 \pm 0.12) \times 10^{-12}$ total rxn; $P = 50-600$ torr Ar	

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$		Notes and Reliability of $\log k$
19,60a	Davis, Bollinger, Fischer (1975)	298	$0.85 \times 10^{-12}$	$P = 3 \text{ torr He}$	total rxn
			$1.36 \times 10^{-12}$	$P = 20 \text{ torr He}$	total rxn
			$1.59 \times 10^{-12}$	$P = 100 \text{ torr He}$	total rxn
	$\text{H}\theta + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{products}$ Perry, Atkinson, Pitts (1977)	298 380-470 298	$(6.40 \pm 0.64) \times 10^{-12}$ $k_1 = 5 \times 10^{-12} \exp(-450/T)$ $k_1/k = 0.16$ (a) $k_1$ refers to H atom abstraction (b) Fraction of rxn proceeding by abstraction; expression for $k_1$ extrapolated to 298K	total rxn; $P = 200 \text{ torr Ar}$ (a) (b)	
19,61	Hansen, Atkinson, Pitts (1975)	298	$(5.78 \pm 0.58) \times 10^{-12}$	total rxn; $P = 100-600 \text{ torr Ar}$	total rxn
	Davis, Bollinger, Fischer (1975)	298	$3.60 \times 10^{-12}$	$P = 3 \text{ torr He}$	total rxn
			$5.00 \times 10^{-12}$	$P = 20 \text{ torr He}$	total rxn
	$\text{H}\theta + \text{CF}_2\text{Cl}_2 \rightarrow \text{products}$ +NASA (1977) eval Atkinson, Hansen, Pitts (1975) Howard, Evenson (1976a) Chang, Kaufman (1977)	200-300 297-424 296 480	$k < 1 \times 10^{-12} \exp(-3560/T)$ $k < 1 \times 10^{-15}$ $k < 4 \times 10^{-16}$ $k < 6 \times 10^{-16}$ (a) upper limit only (b) Expression based on upper limit at 480K reported by Chang and Kaufman. "A factor" chosen; E/R value derived	(a,b) (a) (a) (a)	
19,62	$\text{H}\theta + \text{CFCl}_3 \rightarrow \text{products}$ +NASA (1977) eval Atkinson, Hansen, Pitts (1975) Howard, Evenson (1976a) Chang, Kaufman (1977)	200-300 297-424 296 480	$k < 1 \times 10^{-12} \exp(-3650/T)$ $k < 1 \times 10^{-15}$ $k < 5 \times 10^{-16}$ $k < 5 \times 10^{-16}$ (a) upper limit only (b) Expression based on upper limit at 480K reported by Chang and Kaufman. "A factor" chosen; E/R value derived	(a,b) (a) (a) (a)	
19,63	$\text{H}\theta + \text{CCl}_4 \rightarrow \text{products}$ Howard, Evenson (1976a)	296	$k < 4 \times 10^{-15}$	upper limit only	
19,64	$\text{H}\theta + \text{CH}_2\text{Cl} \rightarrow \text{H}_2\theta + \text{CH}_2\text{Cl}$ +NASA (1977) eval Davis, et al (1976) Perry, Atkinson, Pitts (1976) Howard, Evenson (1976a)	200-300 250-350 298-423 296	$2.2 \times 10^{-12} \exp(-1142/T)$ $(1.84 \pm 0.18) \times 10^{-12} \exp(-1098 \pm 35/T)$ $4.1 \times 10^{-12} \exp(-1359 \pm 150/T)$ $(3.6 \pm 0.8) \times 10^{-14}$	$\pm 0.2 \text{ at } 230\text{K}$	
	$\text{H}\theta + \text{CH}_2\text{Cl}_2 \rightarrow \text{H}_2\theta + \text{CHCl}_2$ +NASA (1977) eval Davis, et al (1976) Perry, Atkinson, Pitts (1976) Howard, Evenson (1976)	200-300 245-375 298 296	$5.2 \times 10^{-12} \exp(-1094/T)$ $(4.27 \pm 0.63) \times 10^{-12} \exp(-1094 \pm 81/T)$ $(1.45 \pm 0.20) \times 10^{-13}$ $(1.55 \pm 0.14) \times 10^{-13}$	$\pm 0.2 \text{ at } 230\text{K}$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
19,64	H $\theta$ + CHCl <sub>3</sub> → H <sub>2</sub> $\theta$ + CCl <sub>3</sub> †Davis, et al (1976)	245-375	(4.69 ± 0.71) x 10 <sup>-12</sup> exp(-1134 ± 108/T)	±0.2 at 230K
19,65	Howard, Evenson (1976a) H $\theta$ + CHFCl <sub>2</sub> → H <sub>2</sub> $\theta$ + CFCl <sub>2</sub> †NASA (1977) eval	296	1.01 ± 0.15 x 10 <sup>-13</sup>	
19,65	Perry, Atkinson, Pitts (1976) Chang, Kaufman (1977) Watson, et al (1977) Howard, Evenson (1976a) H $\theta$ + CHF <sub>2</sub> Cl → H <sub>2</sub> $\theta$ + CF <sub>2</sub> Cl	200-300 298-422 241-396 245-375 296	1.3 x 10 <sup>-12</sup> exp(-1127/T) 1.75 x 10 <sup>-12</sup> exp(-1253 ± 150/T) (1.16 ± 0.17) x 10 <sup>-12</sup> exp(-1073 ± 40/T) (1.87 ± 0.2) x 10 <sup>-12</sup> exp(-1245 ± 26/T) 2.6 x 10 <sup>-14</sup>	±0.2 at 230K
19,65	†NASA (1977) eval Atkinson, Hansen, Pitts (1975) Chang, Kaufman (1977) Watson, et al (1977) Howard, Evenson (1976a) H $\theta$ + CH <sub>2</sub> FCl → H <sub>2</sub> $\theta$ + CHFCl	200-300 297-434 253-427 250-350 296	1.2 x 10 <sup>-12</sup> exp(-1660/T) 1.21 x 10 <sup>-12</sup> exp(-1636 ± 150/T) (1.20 ± 0.16) x 10 <sup>-12</sup> exp(-1657 ± 39/T) (9.25 ± 1.0) x 10 <sup>-13</sup> exp(-1575 ± 71/T) 3.4 x 10 <sup>-15</sup>	±0.2
19,65	†Watson, et al (1977) Howard, Evenson (1976a) H $\theta$ + CH <sub>3</sub> F → products	245-375 296	(2.84 ± 0.3) x 10 <sup>-12</sup> exp(-1259 ± 50/T) 3.7 ± 0.6 x 10 <sup>-14</sup>	
19,65	Howard, Evenson (1976a) H $\theta$ + CH <sub>2</sub> F <sub>2</sub> → products	296	16 ± 2 x 10 <sup>-15</sup>	
19,65	Howard, Evenson (1976a) H $\theta$ + CHF <sub>3</sub> → products	296	7.8 ± 1.2 x 10 <sup>-15</sup>	
19,65	Howard, Evenson (1976a) H $\theta$ + CF <sub>4</sub> → products	296	2 x 10 <sup>-16</sup>	
19,65	Howard, Evenson (1976a) H $\theta$ + CF <sub>3</sub> Cl → products	296	k < 4 x 10 <sup>-16</sup>	upper limit only
19,65	Howard, Evenson (1976a) H $\theta$ + CH <sub>3</sub> Br → H <sub>2</sub> $\theta$ + CH <sub>2</sub> Br	296	k < 7 x 10 <sup>-16</sup>	upper limit only
19,65	†Davis, et al (1976) Howard, Evenson (1976a) H $\theta$ + CH <sub>3</sub> CCl <sub>3</sub> → products	245-350 296	(7.93 ± 0.79) x 10 <sup>-13</sup> exp(-889 ± 98/T) 35 ± 8 x 10 <sup>-13</sup>	±0.2 at 230K
19,65	†NASA (1977) eval Watson, et al (1977) Chang, Kaufman (1977) Howard, Evenson (1976b) H $\theta$ + C <sub>2</sub> HCl <sub>3</sub> → products	200-300 260-375 275-405 296	3.5 x 10 <sup>-12</sup> exp(-1562/T) (3.72 ± 0.4) x 10 <sup>-12</sup> exp(-1627 ± 50/T) (1.95 ± 0.24) x 10 <sup>-12</sup> exp(-1333 ± 37/T) 15 ± 3 x 10 <sup>-15</sup>	±0.36 at 230K
19,65	†NASA (1977) eval Chang, Kaufman (1977) Davis (1977) Howard (1976)	200-300 234-420 300 296	2.3 x 10 <sup>-12</sup> (5.32 ± 0.71) x 10 <sup>-13</sup> exp(+445 ± 41/T) 2.35 ± 0.25 x 10 <sup>-12</sup> 2.0 ± 0.4 x 10 <sup>-12</sup>	±0.36 preliminary



No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Notes and Reliability of log k
19,65	$\text{H}\theta + \text{C}_2\text{Cl}_4 \rightarrow \text{products}$ †*Chang, Kaufman (1977) Davis (1977)	297-420 260-375 296	$(9.44 \pm 1.34) \times 10^{-12} \exp(-1199 \pm 55/T)$ $(1.06 \pm 0.5) \times 10^{-11} \exp(-1300 \pm 150/T)$ $1.70 \times 0.34 \times 10^{-13}$	$\pm 0.36$ at 230K preliminary
19,65	$\text{H}\theta + \text{CH}_3\text{CF}_2\text{Cl} \rightarrow \text{products}$ Howard (1976)			
19,65	Watson, et al (1977) Howard, Evenson (1976b) $\text{H}\theta + \text{CF}_2\text{ClCFCl}_2 \rightarrow \text{products}$	273-375 296	$(1.15 \pm 0.15) \times 10^{-12} \exp(-1748 \pm 30/T)$ $2.8 \pm 0.4 \times 10^{-15}$	
20,M	Watson, et al (1977) $\text{H}\theta_2 + \text{M} \rightarrow \text{H} + \theta_2 + \text{M}$	298	$k < 3 \times 10^{-16}$ see reverse reaction	upper limit only
20,M	$\text{H}\theta_2 + \text{M} \rightarrow \text{H}\theta + \theta + \text{M}$		see reverse reaction	
20,20	$\text{H}\theta_2 + \text{H}\theta_2 \rightarrow \text{H}_2\theta_2 + \theta_2$ †*Hamilton, Lil (1977)	258	$-d[\text{H}\theta_2]/dt = 2k[\text{H}\theta_2]^2$ $2.5 \times 10^{-12}$ (a) Superseded result reported in Hamilton (1975)	$\pm 0.3$ (a)
20,21	Baulch, et al (1972) review Lloyd (1974) review $\text{H}\theta_2 + \text{H}_2 \rightarrow \text{H}_2\theta_2 + \text{H}$	300 300-1000	$3.3 \times 10^{-12}$ $1.7 \times 10^{-11} \exp(-500/T)$ Temperature coefficient	$\pm 0.3$ at 300K larger at higher T
20,22	$\text{H}\theta_2 + \text{H}_2\theta \rightarrow \text{H}_2\theta_2 + \text{H}\theta$ Baulch, et al (1972) review Lloyd (1974) review	300-800 300-1000	$1.2 \times 10^{-12} \exp(-9400/T)$ same recommendation. $k_f = k_r K_{\text{eq}}$	$\pm 0.3$
20,28	$\text{H}\theta_2 + \text{S}\theta_2 \rightarrow \text{S}\theta_3 + \text{H}\theta$ *Payne, Stief, Davis (1973)	300-800 300-1000	$4.7 \times 10^{-11} \exp(-16,500/T)$ same recommendation $k_f = k_r K_{\text{eq}}$	$\pm 0.2$
20,35	$\text{H}\theta_2 + \text{Cl} \rightarrow \text{HCl} + \theta_2$ †*Leu, DeKore (1976)	300	$9 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (a) Relative rate measurement. Value based on $k(\text{H}\theta_2 + \text{H}\theta_2)$ this survey.	$\pm 0.3$ (a)
20,35Br	$\text{H}\theta_2 + \text{Br} \rightarrow \text{HBr} + \theta_2$ †*NASA (1977) eval	200-300	$3 \times 10^{-11}$ (a) estimate - no data	$\pm 0.6$ at 230K $\pm 1.5$ at 230K (a)
20,36	$\text{H}\theta_2 + \text{Cl}\theta \rightarrow \text{H}\theta\text{Cl} + \theta_2$ †*NASA (1977) eval	200-300	$2 \times 10^{-13}$ (a) No data; value assumed to be intermediate between $k(\text{H}\theta_2 + \text{H}\theta_2)$ and $k(\text{Cl}\theta + \text{Cl}\theta)$	$\pm 1$ at 230K (a)
20,45	$\text{H}\theta_2 + \text{C}\theta \rightarrow \text{C}\theta_2 + \text{H}\theta$ *This survey Baulch, et al (1976) review	300 700-1000	$2.5 \times 10^{-10} \exp(-11900/T)$	$\pm 0.5$ a



No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of log k	
				log k	
20,48	Lloyd (1974) eval.	300-1000	$1.7 \times 10^{-13} \exp(-5000/T)$	b	
	Westenberg, deHaas (1972a)	300	$\sim 1 \times 10^{-12}$	c,d	
	Davis, Payne, Stief (1973)	300	$< 10^{-20}$	e	
	Wyrach, et al (1974)	300	$< 3 \times 10^{-18}$	e	
	Simonaitis, Heicklen (1973a)	373-473	$< 5 \times 10^{-18}$	e	
20,51	Volman, Gorse (1972)	330	$< 10^{-15}$	f	
	Baldwin, Walker, Webster (1970)	713-773	$1 \times 10^{-10} \exp(-11500/T)$	e	
	Vardanyan, Dangyan, Sachyan (1972)	878-952	$2.2 \times 10^{-10} \exp(-11500/T)$	e	
NOTE: a. The low value of k selected in this evaluation is based on the evaluation by Lloyd and the measurements by Davis, Payne, Stief and Simonaitis, Heicklen.					
b. Based on Davis, Payne and Stief (1972) and high T results. Temperature coef. probably maximum value.					
c. Indirect measurement using a low-pressure discharge flow system.					
d. Relative rate measurement = reference reaction: $\text{H} + \text{H}\theta_2 \rightarrow \text{H}\theta + \text{H}\theta$					
e. Relative rate measurement = reference reaction: $\text{H}\theta_2 + \text{H}\theta_2 \rightarrow \text{H}_2\theta_2 + \theta_2$					
f. Relative rate measurement = reference reaction: $\text{H}\theta + \text{C}\theta \rightarrow \text{C}\theta_2 + \text{H}$					
20,57	$\text{H}\theta_2 + \text{CH}_2\theta \rightarrow \text{H}_2\theta_2 + \text{CH}\theta$	300-800	$1.7 \times 10^{-12} \exp(-4000/T)$		$> \pm 1$ at 300K, $\pm 0.2$ at 800K
	*Lloyd (1974) review	773	$1.6 \times 10^{-15}$	(a)	
(a) Derived by computer fit to data. Based on $k(\text{H}\theta_2 + \text{H}\theta_2 \rightarrow \text{H}_2\theta_2 + \theta_2) = 3.0 \times 10^{-12} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$					
20,58	$\text{H}\theta_2 + \text{CH}_3\theta_2 \rightarrow \text{CH}_3\theta_2\text{H} + \theta_2$	300	$6.7 \times 10^{-14}$		estimate
	Demerjian et al (1972) review	773	$2.5 \times 10^{-17}$	(a)	
(a) Relative to $k(\text{H}\theta_2 + \text{HCH}\theta) = 1.6 \times 10^{-15}$					
20,59	$\text{H}\theta_2 + \text{C}_2\text{H}_4 \rightarrow \text{addition products}$	300	$\sim 1.7 \times 10^{-17}$		$> \pm 1$ (a)
	Lloyd (1974) review	300-1000		(a) Suggestion. Data are irreconcilable.	
20,60	$\text{H}\theta_2 + \text{C}_2\text{H}_6 \rightarrow \text{H}_2\theta_2 + \text{C}_2\text{H}_5$	300-1000	$\sim 1.7 \times 10^{-12} \exp(-7000/T)$		$\pm 1$ (a)
	Lloyd (1974) review			(a) Relative rate data versus $2\text{H}\theta_2 \rightarrow \text{H}_2\theta_2 + \theta_2$ and $\text{H}\theta_2 + \text{C}\theta \rightarrow \text{H}\theta + \text{C}\theta_2$ . Temp. coef. estimated.	
20,61	$\text{H}\theta_2 + \text{C}_3\text{H}_8 \rightarrow \text{H}_2\theta_2 + 1-\text{C}_3\text{H}_7$	300-1000	$< 3.3 \times 10^{-13} \exp(-5300/T)$		$\pm 1$ (a)
	Lloyd (1974) review				

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k																																													
20,60	$\text{H}\theta_2 + n\text{-C}_4\text{H}_{10} \rightarrow \text{H}_2\theta_2 + s\text{-C}_4\text{H}_9$ (primarily) Lloyd (1974) review	300-1000	(a) Based on upper limit meas. Temp. coef. estimated. $8.7 \times 10^{-13} \exp(-5300/T)$ (a) Based on upper limit meas. Temp. coef. estimated.	$\pm 1$ (a)																																													
20,60	$\text{H}\theta_2 + i\text{-C}_4\text{H}_{10} \rightarrow \text{H}_2\theta_2 + t\text{-C}_4\text{H}_9$ Lloyd (1974) review	300-1000	$1.7 \times 10^{-13} \exp(-3500/T)$ (a) Based on upper limit meas. Temp. coef. estimated.	$\pm 1$ (a)																																													
20,60	$\text{H}\theta_2 + \text{alkane} \rightarrow \text{H}_2\theta_2 + \text{alkyl radical}$ Walker (1977)	300-800	$k = 8 \times 10^{-14} [N_p \exp(-7520/T) + N_s \exp(-6330/T)] + N_t \exp(-4990/T)$ where $N_p$ , $N_s$ , and $N_t$ are the number of primary, secondary, and tertiary hydrogen atoms respectively see reverse reaction																																														
21,M 21,35	$\text{H}_2 + \text{M} \rightarrow \text{H} + \text{H} + \text{M}$ $\text{H}_2 + \text{Cl} \rightarrow \text{HCl} + \text{H}$ † Watson (1977) eval Watson, et al (1977) Lee, et al (1977)	200-300 213-350 200-500	$3.5 \times 10^{-11} \exp(-2290/T)$ ( $5.5 \pm 0.5$ ) $\times 10^{-11} \exp(-2375 \pm 100/T)$ ( $2.66 \pm 0.42$ ) $\times 10^{-11} \exp(-2230 \pm 60/T)$	$\pm 0.12$ at 230K																																													
21,36	$\text{H}_2 + \text{Cl}\theta \rightarrow \text{products}$ † NASA (1977) eval	200-300	$k \leq 1 \times 10^{-12} \exp(-4800/T)$ (a) "A factor" chosen. $F_{\text{act}}$ fitted to upper limit at $T = 670\text{K}$ reported in Watson's review (1977)	$\pm 2$ at 270K (a)																																													
22,29	$\text{H}_2\theta + \text{S}\theta_3 \rightarrow \text{products}$ Castleman, et al (1975)	298	$9.1 \pm 2.9 \times 10^{-13}$																																														
23,hv	$\text{H}_2\theta_2 + h\nu \rightarrow \text{H}\theta + \text{H}\theta$ DeMore (1977)		<table> <tr> <th><math>\Delta/nm</math></th><th><math>10^{20} \frac{x}{\sigma}</math></th><th><math>\Delta/nm</math></th><th><math>10^{20} \frac{x}{\sigma}</math></th><th>(a)</th></tr> <tr><td>200</td><td>48.3</td><td>280</td><td>2.1</td><td></td></tr> <tr><td>210</td><td>36.3</td><td>290</td><td>1.14</td><td></td></tr> <tr><td>220</td><td>26.4</td><td>300</td><td>0.66</td><td></td></tr> <tr><td>230</td><td>18.7</td><td>310</td><td>0.38</td><td></td></tr> <tr><td>240</td><td>12.9</td><td>320</td><td>0.21</td><td></td></tr> <tr><td>250</td><td>8.9</td><td>330</td><td>0.13</td><td></td></tr> <tr><td>260</td><td>5.5</td><td>340</td><td>0.08</td><td></td></tr> <tr><td>270</td><td>3.4</td><td>350</td><td>0.04</td><td></td></tr> </table> <p>(a) <math>\sigma</math> is the absorption cross section in units of <math>\text{cm}^2\text{molecule}^{-1}</math> (base e). These values by DeMore (private communication) are in good agreement (within 10%) with unpublished results by Molina, et al and with results of Holt, et al (1948) over common ranges of measurements</p>	$\Delta/nm$	$10^{20} \frac{x}{\sigma}$	$\Delta/nm$	$10^{20} \frac{x}{\sigma}$	(a)	200	48.3	280	2.1		210	36.3	290	1.14		220	26.4	300	0.66		230	18.7	310	0.38		240	12.9	320	0.21		250	8.9	330	0.13		260	5.5	340	0.08		270	3.4	350	0.04		
$\Delta/nm$	$10^{20} \frac{x}{\sigma}$	$\Delta/nm$	$10^{20} \frac{x}{\sigma}$	(a)																																													
200	48.3	280	2.1																																														
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<p>Hampson (1973) review</p> <p>Quantum yields (primary)</p> <p><math>\phi(-\text{H}_2\theta_2) = 1.0 \quad \lambda &gt; 200\text{nm}</math></p>																																																	

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
23, M	H <sub>2</sub> O <sub>2</sub> + M → HO + HO + M		see reverse equation	
23, 35	H <sub>2</sub> O <sub>2</sub> + Cl → HCl + HO <sub>2</sub>	265-400	1.7 x 10 <sup>-12</sup> exp(-384/T)	±0.36 at 230K
23, 35Br	+Watson (1977) review H <sub>2</sub> O <sub>2</sub> + Br → HBr + HO <sub>2</sub>	200-300	5 x 10 <sup>-12</sup> exp(-1570/T)	±0.6 at 270K
24, M	+NASA (1977) eval HN <sub>3</sub> + M → H + N <sub>3</sub> + M	230-700	5 x 10 <sup>-8</sup> exp(-24,500/T) M = H <sub>2</sub> (a) No data. Value based on reverse rate	±0.2 (a)
24, 24	HN <sub>3</sub> + HN <sub>3</sub> → H <sub>2</sub> O + N <sub>2</sub> O	300	4 x 10 <sup>-15</sup>	±0.3
25, hv	*Baulch, et al (1973) review HN <sub>3</sub> + hv → HO + N <sub>3</sub> (a) → H + N <sub>3</sub> (b)	300	table of absorption cross sections for wavelength range 200-400nm. (a) Gives corrected values which supersede results in Johnston, Graham (1974). Also gives results of Cox and Derwent (1976)	(a)
	Molina (1977) review		table of absorption cross sections for λ = 200-400nm	
	Cox, Derwent (1976)	300	φ <sub>a</sub> ≥ 0.97	(a)
	Cox (1974b)		(a) Photolysis 330 < λ/nm < 380 Elevation/km k(noon)/s <sup>-1</sup> k(24 hr. av.)/s <sup>-1</sup>	
26, hv	HN <sub>3</sub> + hv → HO + N <sub>3</sub>	217	15 5.1 x 10 <sup>-7</sup> 1.5 x 10 <sup>-7</sup>	±0.15
	*Johnston (1974) review	217	20 7.7 x 10 <sup>-7</sup> 2.3 x 10 <sup>-7</sup>	Rates are for 45° latitude
		222	25 2.8 x 10 <sup>-6</sup> 6.8 x 10 <sup>-7</sup>	solar equinox
		227	30 1.4 x 10 <sup>-5</sup> 3.5 x 10 <sup>-6</sup>	standard ozone
		237	35 4.1 x 10 <sup>-5</sup> 1.2 x 10 <sup>-5</sup>	background
		251	40 7.6 x 10 <sup>-5</sup> 2.7 x 10 <sup>-5</sup>	
		265	45 1.1 x 10 <sup>-4</sup> 4.2 x 10 <sup>-5</sup>	
	*Johnston, Graham (1973)		Table of absorption coefficients for λ = 190-325nm	
	Johnston, et al (1974)		φ = 1 200 < λ < 315nm	(a)
	Blaume (1973)		(a) Products probably those shown above. Absorption cross section data for for 185 < λ < 325 nm in good agreement with that of Johnston and Graham (1973). figure showing extinction coefficient vs λ for λ = 120-170nm see reverse reaction	
26, M	HN <sub>3</sub> + M → HO + N <sub>3</sub> + M	200-300	1.0 x 10 <sup>-11</sup> exp(-2170/T)	±0.6 at 230K (a)
26, 35	HN <sub>3</sub> + Cl → HCl + N <sub>3</sub>	295	(6.8 ± 3.4) x 10 <sup>-15</sup> (a) "A factor" chosen. Eact derived to fit room temp. result of Leu, DeMore.	
	+NASA (1977) eval Leu, DeMore (1976)			

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
226a, 34b	S + CS <sub>2</sub> → S <sub>2</sub> + CS	298	6.5 x 10 <sup>-13</sup>	±0.2
26a, 34c	Baulch, et al (1976) review S + COS → CS + S <sub>2</sub>	230-2600	2.8 x 10 <sup>-12</sup> exp(-2050/T)	±0.5
27, 27	Baulch, et al (1976) review S $\dot{O}$ + S $\dot{O}$ → S $\dot{O}_2$ + S or (S $\dot{O}$ ) <sub>2</sub>	300 1000 300	< 3 x 10 <sup>-15</sup> < 2 x 10 <sup>-13</sup> 8.3 ± 6.7 x 10 <sup>-16</sup>	
27, 29	Schofield (1973) review Chung, Calvert, Bottenheim (1975) S $\dot{O}$ + S $\dot{O}_3$ → 2S $\dot{O}_2$	300	2 ± 1.2 x 10 <sup>-15</sup>	
28, 49M	Chung, Calvert, Bottenheim (1975) S $\dot{O}_2$ + CH <sub>3</sub> (•M) → CH <sub>3</sub> S $\dot{O}_2$ (•M)	300	3 x 10 <sup>-13</sup> cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	±0.1
31, 31	James, et al (1973) HS + HS → H <sub>2</sub> S + S	295	1.2 x 10 <sup>-11</sup>	±0.2
35, 35M	Baulch, et al (1976) review Cl + Cl + M → Cl <sub>2</sub> + M	200-500	6 x 10 <sup>-34</sup> exp(900 ± 250/T) cm <sup>6</sup> molecule <sup>-2</sup> s <sup>-1</sup> M = Ar	±0.1
35, 37	*Watson (1977) review Cl + OCl $\dot{O}$ → 2Cl $\dot{O}$	300-588	(5.9 ± 0.9) x 10 <sup>-11</sup> exp(0 ± 120/T)	
35, 37	*Watson (1977) review Cl + Cl $\dot{O}$ → Cl <sub>2</sub> + $\dot{O}_2$ (a) → 2Cl $\dot{O}$ (b)		k <sub>a</sub> = 1.6 x 10 <sup>-10</sup> k <sub>b</sub> = 1.1 x 10 <sup>-11</sup> k <sub>a</sub> = 1.56 x 10 <sup>-10</sup> k <sub>a</sub> /k <sub>b</sub> = 108 k <sub>a</sub> /k <sub>b</sub> = 15	
35, 44a	*NASA (1977) eval Johnston, et al (1969)	298	6.8 x 10 <sup>-13</sup>	
35, 44a	Nicholas, Norrish (1968) Cl + Cl <sub>2</sub> $\dot{O}$ → Cl <sub>2</sub> + Cl $\dot{O}$	258	3 ± 0.5 x 10 <sup>-11</sup>	
35, 42	*Watson (1977) review Cl + NOCl → NO + Cl <sub>2</sub>	300	k >> 3 x 10 <sup>-14</sup>	
35, 43	*Watson (1977) review Cl + NO <sub>2</sub> Cl → NO <sub>2</sub> + Cl <sub>2</sub>	258	1.68 x 10 <sup>-12</sup> exp(-607/T)	±0.3
35, 43a	Watson (1977) review Cl + NO <sub>3</sub> Cl → products	298	7.3 x 10 <sup>-12</sup> exp(-1269/T)	(a)
35, 56	*Kurylo, Manning (1977) Cl + CB <sub>4</sub> → HCl + CH <sub>3</sub>	224-273	(7.93 ± 1.53) x 10 <sup>-12</sup> exp(-1273 ± 51/T)	(b)
35, 56	*Watson (1977) review Manning, Kurylo (1977)	200-300	(7.94 ± 0.7) x 10 <sup>-12</sup> exp(-1260 ± 35/T)	
35, 56	Watson, et al (1976)	218-401	5.44 x 10 <sup>-19</sup> T <sup>2.50</sup> exp(-608/T)	
35, 56	Whytock, et al (1977)	200-299	(6.51 ± 0.79) x 10 <sup>-12</sup> exp(-1229 ± 27/T)	
35, 56	Zahniser, et al (1978)	200-500	8.6 x 10 <sup>-18</sup> T <sup>2.11</sup> exp(-795/T)	
35, 56	Davis, et al (1970)	200-300	(8.2 ± 0.6) x 10 <sup>-12</sup> exp(-1320 ± 20/T)	
35, 56		300	1.5 ± 0.1 x 10 <sup>-13</sup>	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	Notes and Reliability of log k
35,58	Fettis, Knox (1964) Clyne, Walker (1973)	300-686	$4 \times 10^{-11} \exp(-1930/T)$ $5.1 \times 10^{-11} \exp(-1790/T)$ (a) Based on four direct 1976, 1977 studies listed immediately below. Uncertainty in log k(230K) is $\pm 0.12$ and $-0.36$ (b) Value changed subsequent to publication to allow for effect of small $\text{C}_2\text{H}_6$ impurity see Watson's review (1977)	
36,hv	$\text{Cl} + \text{C}_2\text{H}_6 \rightarrow \text{HCl} + \text{C}_2\text{H}_5$ Manning, Kurylo (1977) $\text{Cl}\dot{\theta} + \text{h}\nu \rightarrow \text{Cl} + \dot{\theta}$ *Watson (1977) review	22-322	$(7.29 \pm 1.23) \times 10^{-11} \exp(-60 \pm 44/T)$ absorption cross section data $225 < \lambda < 300 \text{ nm}$	
36,36	$\text{Cl}\dot{\theta} + \text{Cl}\dot{\theta} \rightarrow \text{Cl} + \text{Cl}\dot{\theta}\dot{\theta}$ (a) $\rightarrow \text{Cl}_2 + \dot{\theta}_2$ (b) $\rightarrow \dot{\theta}\text{Cl}\dot{\theta} + \text{Cl}$ (c) †*NASA (1977) eval	200-300	$k_a = 1 \times 10^{-12} \exp(-1238/T)$ $k_b = 5 \times 10^{-13} \exp(-1238/T)$ $k_c = 2 \times 10^{-12} \exp(-2200/T)$ (a) $-d[\text{Cl}\dot{\theta}]/dt = k[\text{Cl}\dot{\theta}]^2$ . Low pressure. See Watson's review (1977) for high pressure rec.	$\pm 0.2$ at 230K (a) $\pm 0.2$ at 230K $\pm 1$ at 230K
36,36Br	$\text{Cl}\dot{\theta} + \text{Br}\dot{\theta} \rightarrow \text{Br} + \dot{\theta}\text{Cl}\dot{\theta}$ (a) $\rightarrow \text{Br} + \text{Cl}\dot{\theta}\dot{\theta}$ (b) †*Watson (1977) review		$k_a = (6.7 \pm 1.0) \times 10^{-12}$ $k_b = (6.7 \pm 1.0) \times 10^{-12}$	$\pm 0.36$ at 230K $\pm 0.36$ at 230K
36,45	$\text{Cl}\dot{\theta} + \text{O}\dot{\theta} \rightarrow \text{O}\dot{\theta}_2 + \text{Cl}$ †*NASA (1977) eval	200-300	$k \leq 1 \times 10^{-12} \exp(-3700/T)$ (a) "A factor" chosen. $E_{\text{act}}$ fitted to upper limit at $T = 587\text{K}$ reported in Watson's review (1977)	$\pm 2$ at 230K (a)
36,56	$\text{Cl}\dot{\theta} + \text{CH}_4 \rightarrow \text{products}$ †*NASA (1977) eval	200-300	$k \leq 1 \times 10^{-12} \exp(-3700/T)$ (a) "A factor" chosen. $E_{\text{act}}$ fitted to upper limit at $T = 670\text{K}$ reported in Watson's review (1977)	$\pm 2$ at 230K (a)
36,57	$\text{Cl}\dot{\theta} + \text{C}_2\text{H}_4 \rightarrow \text{products}$ Walker (1972)	670	$k < 5 \times 10^{-16}$ (a) AS quoted by Watson (1977) review.	(a)
36,59	$\text{Cl}\dot{\theta} + \text{C}_2\text{H}_2 \rightarrow \text{products}$ Walker (1972)	670	$k < 5 \times 10^{-16}$ (a) AS quoted by Watson (1977) review.	(a)
36Br,36Br	$\text{Br}\dot{\theta} + \text{Br}\dot{\theta} \rightarrow 2\text{Br} + \dot{\theta}_2$ †*NASA (1977) eval Clyne, Watson (1975) Clyne, Cruse (1970)	200-300 298 293	$2.9 \times 10^{-11} \exp(-450/T)$ $6.4 \times 10^{-12}$ $5.3 \times 10^{-11} \exp(-450/T)$	$\pm 0.36$ at 230K



No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
37, M	ClO <sub>2</sub> + M → Cl + O <sub>2</sub> + M Watson (1977) review			Table of values of rate constant as a function of altitude.
37, hv	ClO <sub>2</sub> + hv → ClO + O Watson (1977) review		absorption cross section data 225 < λ < 280 nm	
37, hv	ClO <sub>2</sub> + hv → ClO + O Watson (1977) review		Abs. cross section data 150 < λ < 480nm	
39, hv	HCl + hv → H + Cl Watson (1977) review		absorption cross section data 140 < λ < 220 nm	
40, hv	H <sub>2</sub> O + hv → products Watson (1977) review		Abs. cross section data 290 < λ < 450nm	
42, hv	NOCl + hv Molina (1977) review		Table of absorption cross section values for λ = 190-400nm	
43, hv	ClNO <sub>2</sub> + hv Molina (1977) review		Absorption cross section data for λ = 190-400nm	
43, hv	ClONO <sub>2</sub> + hv Molina (1977)		Absorption cross section data for λ = 235-400nm	
43a, hv	NO <sub>3</sub> Cl + hv Rowland, Spencer, Molina (1976)			Table of absorption cross section values for λ = 186-460nm. Also table of solar photodissociation coefficients Data also tabulated in reviews by Watson (1977) and by Molina (1977). Molina's review also discusses quantum yield data
44, hv	Cl <sub>2</sub> + hv → 2Cl Watson (1977) review		absorption cross section data 240 < λ < 450 nm see CH <sub>3</sub> O + CO	
45, 50	CO + CH <sub>3</sub> → . . .			
48, hv	CH <sub>2</sub> O + hv → CH <sub>2</sub> O* → H + HCO (1) → H <sub>2</sub> + CO (2) This survey (1978)			
			λ/nm	g <sub>1</sub> g <sub>2</sub> 0.90
			285	0.61
			290	0.74
			295	0.74
			300	0.74
			305	0.74
			310	0.74
			315	0.74
			320	0.60
			325	0.45
			330	0.31

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
335			0.17	1
340			0.02	0.64
Tentative recommendation based principally on results reported by Horowitz and Calvert (1978a) and by Moortgat, et al (1978). Also considers results reported in Clark, Moore and Nogar (1977), Horowitz and Calvert (1978b), Houston and Moore (1976), Lewis and Lee (1977), Lewis, Tang and Lee (1976) and Marling (1977).				
Apparent quantum yield values are slightly higher in presence of O <sub>2</sub> . Effect is assumed here to be due to secondary reactions.				
	Calvert, et al (1972)		$\frac{\Delta/nm}{10^{20}} \frac{x}{\sigma}$	$\frac{\Delta/nm}{10^{20}} \frac{x}{\sigma}$ (a)
290			3.18	330
300			3.25	340
310			3.14	350
320			2.34	360
(a)	$\sigma$ is the value of the absorption cross section averaged for 10nm bands. See McQuigg, Calvert (1969) for figure of of absm. coeff. vs wave length. Also see Miller and Lee (1977) for higher resolution spectra from which absorption cross section values can be derived.			
50.4	CH <sub>3</sub> θ + θ <sub>2</sub> → CH <sub>2</sub> θ + Hθ <sub>2</sub> (1)			
50.9	CH <sub>3</sub> θ + Nθ → CH <sub>3</sub> θNθ (2a) → CH <sub>2</sub> θ + HNθ (2b)			
50.10	CH <sub>3</sub> θ + Nθ <sub>2</sub> → CH <sub>3</sub> θNθ <sub>2</sub> (3a) → CH <sub>2</sub> θ + HNθ <sub>2</sub> (3b)			
50.45	CH <sub>3</sub> θ + Cθ → products (4)			
	*Heicklen (1973)	258	k <sub>1</sub> ~ 3 x 10 <sup>-18</sup> ~ 1.6 x 10 <sup>-13</sup> exp(-3300/T)	
		298	k <sub>2</sub> ~ 8 x 10 <sup>-14</sup> k <sub>1</sub> /k <sub>2</sub> = 4.7 x 10 <sup>-5</sup> ±20%	ratio probably is smaller at 220K
298			k <sub>2b</sub> /k <sub>2</sub> = 0.145 ±0.015	
363			k <sub>2</sub> /k <sub>3</sub> = 1.2 ±0.1	
403			k <sub>2a</sub> /k <sub>3a</sub> = 1.1 = 1.8	
258			= 2.7	
258			k <sub>3a</sub> /k <sub>3</sub> = 0.9 ±0.1	
258			k <sub>3b</sub> /k <sub>3</sub> = 0.1 ±0.01	
298-423			k <sub>4</sub> /k <sub>2</sub> = 5 x 10 <sup>-4</sup>	* k <sub>3a</sub> /k <sub>3b</sub> probably constant ±00-400K
300-400	Demerjian, et al (1974) review		k <sub>1</sub> = 1.6 x 10 <sup>-17</sup>	

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Notes and Reliability of log k
$\sim 4.2 \times 10^{-13} \exp(-3000/T)$ adjusted to fit C <sub>4</sub> H <sub>10</sub> /N <sub>2</sub> simulation studies				
51, 51	Batt, McCulloch, Milne (1975)  Barker, et al (1977) 2CH <sub>3</sub> • → 2CH <sub>3</sub> • + • (a) → CH <sub>3</sub> • + CH <sub>2</sub> • + • (b) → CH <sub>3</sub> • + CH <sub>2</sub> • + • (c)  Weaver, et al (1975)	393-473  396-442	$k_{2a} = 1.7 \times 10^{-13}$ $k_{2b}/k_{2a} = 0.17$ $k_{3a} = 3.3 \times 10^{-13}$ $k_{3b}/k_{3a} = 0.1$ $k_{2a} \sim 3 \times 10^{-11}$ $k_{2b} \sim 7 \times 10^{-12}$ $k_1 = 5 \times 10^{-13} \exp(-2000/T)$	±0.4 ±0.5
54, hv	Parkes (1977)  CH <sub>3</sub> • + hv → CH <sub>3</sub> • + N• (a) → isomer (b) → CH <sub>2</sub> • + H• (c) → CH <sub>2</sub> • + H• + N• (d)  *Heicklen (1973) review	300	$k_a/k = 0.43$ $k_b/k = 0.50$ $k_c/k = 0.07$ $k_a = 1.6 \pm 0.4 \times 10^{-13}$ $k_b + k_c = 3.0 \pm 0.8 \times 10^{-13}$	
61, hv	CF <sub>2</sub> Cl <sub>2</sub> + hv Watson (1977) review	298 298 298	$k_a/k = 0.76 \pm 0.02, \lambda = 366\text{nm}$ $k_b/k = 0.24 \pm 0.04, \lambda = 366\text{nm}$ $(k_c + k_d)/k < 0.02, \lambda = 366\text{nm}$ $k = k_a + k_b + k_c + k_d$	
62, hv	CFCl <sub>3</sub> + hv Molina (1977) review Watson (1977) review		Absorption cross section data for $174 < \lambda/\text{nm} < 220$ Low temperature absorption cross section data	
63, hv	CCl <sub>4</sub> + hv Molina (1977) review Watson (1977) review		Tabulated values of absorption cross sections for $174 < \lambda/\text{nm} < 230$ . Low temperature abs. cross section data	
			Absorption cross section data for $174 < \lambda/\text{nm} < 238$ . see Watson's review (1977)	

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## APPENDIX 1.

### Chemical Thermodynamic Properties of Selected Molecular Species

E. S. Domalski, D. Garvin, and D. D. Wagman

Two tables are provided showing chemical thermodynamic properties of selected molecular species of interest in stratospheric chemistry. In these tables there are sufficient data for the usual calculations of heats of reaction and equilibria.

The first table lists enthalpy and Gibbs energy of formation, entropy and heat capacity data. The information was extracted from "Selected Values of Chemical Thermodynamic Properties" (D. D. Wagman, et al, NBS Technical Note 270-3, January 1968) except as indicated in the Notes. The thermodynamic properties tabulated are:

1. enthalpy of formation at 0K and 298.15K,
2. Gibbs energy of formation at 298.15K,
3. enthalpy increment between 0K and 298.15K,
4. entropy at 298.15K,
5. heat capacity at constant pressure at 298.15K.

The values given for the heats of formation are based on experimental thermodynamic and spectroscopic measurements except where otherwise indicated; the values of  $S^\circ$ ,  $C_p^\circ$  and  $H_{298}^\circ - H_0^\circ$  for gaseous species were calculated by standard statistical-mechanical equations, using corrections for vibrational anharmonicities, rotational stretching, and rotation-vibration interactions where these data were available.

The second table presents bond dissociation energies or bond strengths. These usually are the enthalpies of simple bond scission reactions. However, there are some cases in which there is a substantial contribution from rearrangement of electronic structure in the products (reducing the bond energy).

The values given here for some molecules may differ slightly from values adopted by the CODATA Task Group on Key Values for Thermodynamics (see CODATA Bulletin 17, published by the International Council of Scientific Unions Committee on Data for Science and Technology, January 1976). These differences will have no significant effect on the enthalpies or free energies of reaction calculated from the tables.

National Bureau of Standards

CHEMICAL THERMODYNAMIC PROPERTIES OF SELECTED MOLECULAR SPECIES

Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity *							
Substance		$\Delta H_f^\circ$	$\Delta H_f^\circ$	$\Delta G_f^\circ$	$H_{298}^\circ - H_0^\circ$	$S^\circ$	$C_p^\circ$
Formula and Description		State	Formula Weight	298.15°K (25°C)			
				0°K	kcal/mol		
O oxygen, atomic	g	15.9994	58.983	59.553	55.389	1.607	38.467
O( <sup>1</sup> D)	g	15.9994	104.34	104.78		1.481	
O( <sup>1</sup> S)	g	15.9994	155.60	156.04		1.481	
O <sub>2</sub> oxygen, molecular, ( <sup>3</sup> Σ <sub>g</sub> <sup>-</sup> )	g	31.9988	0	0	0	2.0746	7.016
O <sub>2</sub> ( <sup>1</sup> Δ)	g	31.9988	22.54	22.54			
O <sub>2</sub> ( <sup>1</sup> Σ)	g	31.9988	37.51	37.51			
O <sub>3</sub> ozone	g	47.9982	34.74	34.1	39.0	2.4736	57.08
H hydrogen, atomic	g	1.0080	51.633	52.103	48.588	1.481	27.391
H <sub>2</sub> hydrogen, molecular	g	2.0159	0	0	0	2.0238	31.208
OH hydroxyl	g	17.0074	9.25	9.31	8.18	2.1070	43.890
HO <sub>2</sub> hydroperoxy 1	g	33.0068	1.2+2	0.5+2	3.4	2.39	54.73
H <sub>2</sub> O water	g	18.0153	-57.102	-57.796	-54.634	2.3667	45.104
H <sub>2</sub> O <sub>2</sub> hydrogen peroxide	g	34.0147	-31.08	-32.58	-25.24	2.594	55.6
N nitrogen, atomic	g	14.0067	112.534	112.979	108.883	1.481	36.622
N <sub>2</sub> nitrogen, molecular	g	28.0134	0	0	0	2.072	45.77
NO nitric oxide	g	30.0061	21.45	21.57	20.69	2.197	50.347
NO <sub>2</sub> nitrogen dioxide	g	46.0055	8.60	7.93	12.26	2.438	57.35
NO <sub>3</sub> nitrogen trioxide	g	62.008	18.5	17.0	27.7	2.62	60.4
N <sub>2</sub> O nitrous oxide	g	44.0128	20.435	19.61	24.90	2.284	52.52
N <sub>2</sub> O <sub>4</sub> dinitrogen tetroxide	g	92.0110	4.49	2.19	23.38	3.918	72.70
							18.47

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## National Bureau of Standards

Washington, D. C.

## Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Substance		Formula Weight	State	$\Delta H_f^\circ$ 0°K	$\Delta H_f^\circ$	$\Delta G_f^\circ$	$H_{298}^\circ - H_0^\circ$	S°	C <sub>p</sub> °
Formula and Description									
				0°K	kcal/mol		298.15°K (25°C)		
							cal/deg mol		
N <sub>2</sub> O <sub>5</sub> dinitrogen pentoxide	g	108.0104	5.7	2.7	27.5	4.237	85.0	20.2	
NH imino (imidogen)	g	15.0147	82.	82.	80.6	2.060	43.29	6.97	
NH <sub>2</sub> amino	g	16.0226	46.2	45.5	47.8	2.37	46.51	8.02	
NH <sub>3</sub> ammonia	g	17.0306	-9.31	-10.98	-3.93	2.40	46.05	8.38	
HNO nitroxyl hydride	g	31.0142	24.5	23.8	26.859	2.387	52.729	8.279	
HNO <sub>2</sub> cis, nitrous acid	g	47.0135	-17.12	-18.64	-10.27	2.608	59.43	10.70	
trans, nitrous acid	g	47.0135	-17.68	-19.15	-10.82	2.652	59.54	11.01	
cis-trans mixture, equil.	g	47.0135	-29.94	-19.0	-11.0		60.7	10.9	
HNO <sub>3</sub> nitric acid	g	63.0129	-29.94	-32.28	-17.87	2.815	63.64	12.75	
S sulfur, rhombic	c	32.064	0	0	0	1.054	7.60	5.41	
	g	32.064	65.7	66.20	56.52	1.591	40.085	5.658	
SO monosulfur monoxide	g	48.0634	1.2	1.2	-5.0	2.087	53.02	7.21	
SO <sub>2</sub> sulfur dioxide	g	64.0628	-70.33	-70.94	-71.74	2.521	59.30	9.53	
SO <sub>3</sub> sulfur trioxide	c	80.0622		-108.63	-88.19		12.5		
	liq	80.0622		-105.41	-88.04		22.85		
	g	80.0622	-93.21	-94.58	-88.69	2.796	61.34	12.11	
H <sub>2</sub> SO <sub>4</sub> sulfuric acid	c	98.0775	-194.069						
	liq	98.0775		-194.548	-164.938	6.748	37.501	33.20	
S <sub>2</sub> O disulfur monoxide	g	80.1274				2.66	63.8	10.5	
HS sulfur monohydride	g	33.0720	33.1	33.3	26.3	2.22	46.73	7.76	

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## Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Substance		State	Formula Weight	$\Delta H_f^\circ$	$\Delta H_f^\circ$	$\Delta G_f^\circ$	$H_{298}^\circ - H_0^\circ$	$S^\circ$	$C_p^\circ$
Formula and Description									
298.15°K (25°C)									
				0°K	kcal/mol			cal/deg mol	
H <sub>2</sub> S	hydrogen sulfide	g	34.0799	-4.232	-4.93	-8.02	2.379	49.16	8.18
C	graphite, Acheson spectroscopic	c	12.0112	0	0	0	0.251	1.372	2.038
CO	carbon monoxide	g	28.0106	-27.199	-26.416	-32.780	2.0716	47.219	6.959
CO <sub>2</sub>	carbon dioxide	g	44.0100	-93.963	-94.051	-94.254	2.2378	51.06	8.87
CH <sub>3</sub>	methyl	g	15.0351	35.6	34.8	35.3	2.49	46.38	9.25
CH <sub>4</sub>	methane	g	16.0430	-15.970	-17.88	-12.13	2.388	44.492	8.439
HCO	formyl	g	29.0185	8.9	9.0	5.36	2.386	53.68	8.26
HCHO	formaldehyde	g	30.0265	-25.03	-25.95	-24.51	2.394	52.26	8.46
CH <sub>3</sub> O	methoxy	g	31.0345	5.8	3.9	6.4	2.41	64.2	8.9
CH <sub>3</sub> O <sub>2</sub>	methylperoxy1	g	47.0339		6.7				
CH <sub>3</sub> OOH	methylhydroperoxide	g	48.0347		-30.8	-17.4		67.9	15.
CH <sub>3</sub> NO <sub>2</sub>	nitromethane	g	61.0406	-14.546	-17.86	-1.65	3.083	65.69	13.70
CH <sub>3</sub> ONO	methyl nitrite	g	61.0406	-13.5	-16.5	-1.5	3.36	69.7	16.5
CH <sub>3</sub> NO <sub>3</sub>	methyl nitrate	g	77.0400	-25.9	-29.8	-9.4	3.55	76.1	16.1
COCl <sub>2</sub>	phosgene	g	98.9166	-52.195	-52.61	-49.20	3.067	67.74	13.78

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# SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES - SERIES 1

National Bureau of Standards

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity						
Substance		$\Delta H_f^\circ$	$\Delta H_f^\circ$	$\Delta G_f^\circ$	$H_{298}^\circ - H_0^\circ$	$S^\circ$
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)		
				kcal/mol		cal/deg mol
$C_2H_2$ acetylene	g	26.0382	54.324	54.19	50.00	48.00
$C_2H_4$ ethylene	g	28.0542	14.515	12.49	16.28	52.45
$C_2H_5$ ethyl radical	g	29.0627		25.7	32.0	59.6
$C_2H_6$ ethane	g	30.0701	-16.323	-20.04	-7.66	54.85
$C_3H_6$ propylene	g	42.0816	8.467	4.88	15.00	63.80
$C_3H_8$ propane	g	44.0976	-19.684	-25.02	-5.81	64.51
$C_4H_{10}$ n-butane	g	58.1248	-23.552	-30.03	-3.97	74.12
$C_4H_{10}$ isobutane	g	58.1248	-25.223	-32.07	-4.91	70.42
$CH_2CO$ ketene	g	42.0376	-10.66	-11.4	-11.6	59.16
$CH_3CO$ acetyl radical	g	43.0456		-5.8	-3.0	64.5
$CH_3CHO$ acetaldehyde	g	44.0536	-37.14	-39.72	-30.31	59.8
$CH_3COC1$ acetyl chloride	g	78.4986	-57.93	-60.07	-51.08	70.56
$Cl$ chlorine, atomic	g	35.453	28.59	28.992	25.173	39.457
$ClO$ chlorine monoxide	g	51.4524	24.33	24.47	23.68	53.78
$ClO_2$ chlorine dioxide (sym.)	g	67.4518	25.09	24.5	28.8	61.36

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SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES - SERIES I

National Bureau of Standards

Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity								
Substance		$\Delta H_f^\circ$	$\Delta H_f^\circ$	$\Delta G_f^\circ$	$H_{298}^\circ - H_0^\circ$	$S^\circ$	$C_p^\circ$	
Formula and Description		State	Formula Weight	298.15°K (25°C)			cal/deg mol	
				0°K	kcal/mol			
ClO <sub>2</sub> chlorine dioxide (unsym.)	g	67.4518	21.7	21.3	25.1	2.78	63.0	11.0
ClO <sub>3</sub> chlorine trioxide	g	83.4512		37				
HCl hydrogen chloride	g	36.4610	-22.020	-22.062	-22.777	2.066	44.646	6.96
HOCl hypochlorous acid	g	52.4604	-18.0	-18.7	-15.7	2.440	56.54	8.88
NOCl nitrosyl chloride	g	65.4591	12.81	12.36	15.77	2.716	62.52	10.68
NO <sub>2</sub> Cl nitryl chloride	g	81.4585	4.29	3.0	13.0	2.915	65.02	12.71
NO <sub>3</sub> Cl chlorine nitrate	g	97.458		6.28				
Cl <sub>2</sub> chlorine, molecular	g	70.906	0	0	0	2.193	53.288	8.104
Cl <sub>2</sub> O dichlorine monoxide	g	86.9054	19.62	19.20	23.3	2.806	64.07	11.48
Cl <sub>2</sub> O <sub>4</sub> chlorine perchlorate	g	134.9036				4.16	78.21	20.56
CF <sub>4</sub> carbon tetrafluoride	g	88.0048	-221.61	-223.04	-212.37	3.043	62.45	14.59
CClF <sub>3</sub> chlorotrifluoromethane	g	104.4594	-168.0	-169.2	-159.5	3.294	68.17	15.99
CF <sub>2</sub> Cl <sub>2</sub> dichlorodifluoromethane	g	120.9140	-116.5	-117.5	-108.2	3.553	71.91	17.31
CCl <sub>3</sub> F trichlorofluoromethane	g	137.3686	-68.24	-69.0	-59.6	3.838	74.00	18.65
CCl <sub>4</sub> carbon tetrachloride	g	153.8232	-22.42	-22.94	-12.83	4.120	74.02	19.93

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# SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES - SERIES I

National Bureau of Standards

Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity											
Table	Substance		Formula Weight	State	Formulation	ΔHf°	ΔHf°	ΔGf°	H298° - H0°	S°	Cp°
	Formula and Description										
	CH3Cl	methyl chloride	g	50.4881	-17.69	-19.59	-13.98	2.489	55.99	9.73	
	CH2Cl2	methylene dichloride	g	84.9331	-21.19	-22.83	-16.49	2.830	64.57	12.16	
	CHCl3	chloroform	g	119.3781	-23.49	-24.66	-16.83	3.383	70.63	15.63	
	CF3	trifluoromethyl radical	g	69.0064	-111.7	-112.4	-109.21	2.754	63.33	11.90	
	CCl3	trichloromethyl radical	g	118.3702	19.15	19.	22.09	3.392	70.92	15.21	
	C2Cl4	tetrachloroethylene	g	165.8343	-2.83	-2.97	5.15	4.759	82.05	22.84	
	C2HCl3	trichloroethylene	g	131.3893	-1.032	-1.86	4.31	3.975	77.6	19.18	
	CH3CCl3	1,1,1-trichloroethane	g	133.4052	-34.65	-34.01	-18.21	4.30	76.49	22.07	
		(methyl chloroform)									

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## Notes

1. Hampson, R. F. et al, J. Phys. Chem. Ref. Data 2, 267-312 (1973)  
[Data sheet on  $O_3 + h\nu$  (u.v.)] p. 303.
2. Contributions of the higher electronic states of molecular oxygen to the enthalpy, entropy, and heat capacity at 298 K are insignificant.
3. Stull, D. R. and Prophet, H. "JANAF Thermochemical Tables" 2nd. ed. NSRDS-NBS 37 (1971).
4. Tsang, W. Estimated from kinetic data on the decomposition of  $N_2H_4$ . Chapter 12, NBS Report 10904, 1 July 1972.
5. NBS Report 10904, 1 July 1972, pp. 239-307.
6. R. A. Fletcher and G. Pilcher, Trans Faraday Soc. 66, 794-799 (1970) provide more recent data for  $\Delta H_f^\circ$ , 298.15 K.
7. Data obtained from Benson and O'Neal ("Kinetic Data on Gas Phase Unimolecular Reactions", NSRDS-NBS-21, Feb 1970, page 55).
8. Heat formation value from S. W. Benson "Thermochemical Kinetics" Second Edition, John Wiley and Sons (1976).
9. Values for  $\Delta H_f^\circ$ ,  $S^\circ$ , and  $C_p^\circ$  at 298.15 K were calculated using the group additivity method described by Benson and O'Neal ("Kinetic Data on Gas Phase Unimolecular Reactions", NSRDS-NBS-21, Feb. 1970, pp. 40-42).

10. The value for  $\Delta H_f^\circ [\text{CH}_3\text{ONO}(\text{g})] = -16.5 \text{ kcal mol}^{-1}$  was derived from the combustion data of Geiseler and Thierfelder (Z. physik. Chem., N. F., 29, 248-257 (1961)), and the equilibrium data of Leermakers and Ramsperger (J. Am. Chem. Soc. 54, 1837-1845 (1932)) for:  $\text{CH}_3\text{OH}(\text{g}) + \text{NOCl}(\text{g}) = \text{CH}_3\text{ONO}(\text{g}) + \text{HCl}(\text{g})$ .
11. The value for  $\Delta H_f^\circ (\text{CH}_3\text{ONO}_2(\text{g})) = -29.8 \text{ kcal mol}^{-1}$  was derived from the work of Ray and Ogg (J. Phys. Chem. 63, 1522-1523 (1959)) on the enthalpy of reaction of  $\text{N}_2\text{O}_5$  with  $\text{CH}_3\text{ONO}$ .
12. We have chosen  $S^\circ [\text{CH}_3\text{ONO}_2(\text{g})] = 76.1 \text{ cal mol}^{-1}\text{K}^{-1}$  based upon low temperature thermal data of Gray and Smith (J. Chem. Soc. 1953, 2380-2385). Calculations from microwave studies by Dixon and Wilson (J. Chem. Phys. 35, 191-198 (1961)) give  $S^\circ = 72.15 \text{ cal mol}^{-1}\text{K}^{-1}$ .
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14. Data on  $\Delta H_f^\circ$ ,  $S^\circ$ ,  $C_p^\circ$  obtained from S. W. Benson and H. E. O'Neal ("Kinetic Data on Gas Phase Unimolecular Reactions", NSRDS-NBS-21, Feb. 1970, page 567).
15. Rossini, F. D., Pitzer, K. S., Arnett, R. L., Braun, R. M. and Pimentel, G. C., "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds", API Research Project 44, Carnegie Press, Pittsburgh, 1953.

16.  $\Delta H_f^\circ$  data from Pittam and Pilcher (J. Chem. Soc., Faraday Trans. I, 68, 2224-2229 (1972)).
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19. Data on  $S^\circ$  and  $C_p^\circ$  were obtained from Note (14), page 589; data on  $\Delta H_f^\circ$  came from Note (18).
20. Spectroscopic studies of N. Basco and R. D. Morse, J. Molec. Spectros. 45, 35 (1973); R. A. Durie and D. A. Ramsay, Can. J. Phys. 36, 35 (1958); P. A. G. O'Hare and A. C. Wahl, J. Chem. Phys. 54, 3770 (1971); L. Andrews and J. I. Raymond, J. Chem. Phys. 55, 3087 (1971); D. R. Johnson and F. X. Powell, Bull. Am. Phys. Soc. 13, 594 (1968); A. Carrington, P. N. Dyer, and D. H. Levy, J. Chem. Phys. 47, 1756 (1967) were examined and used to calculate the thermodynamic properties.
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22. Studies by D. J. Gardiner, J. Mol. Spectroscopy 38, 476 (1971) and G. E. Herberich, R. H. Jackson, and D. J. Miller, J. Chem. Soc. (A) 1966, 336 were examined and the data used to calculate the thermodynamic properties.



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26. The vaporization data of D. L. Hildenbrand and R. A. McDonald, *J. Phys. Chem.* 63, 1521-1522 (1959) were used.
27. The combustion data of R. A. Fletcher and G. Pilcher, *Trans. Faraday Soc.* 67, 3191-3201 (1971) were used to calculate  $\Delta H_f^\circ [\text{CH}_3\text{Cl(g)}]$ .
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32. JANAF Thermochemical Tables Supplement No. 48, June 1977.
33. Heat of formation value based on data in H. D. Knauth, H. Martin and W. Stockmann, Z. Naturforsch. 29A, 200 (1974).
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Bond Dissociation Energies,  $D_0^\circ$  at 0 K  
Calculated from heats of formation in the accompanying table

Reaction	kJ/mol	kcal/mol	Note
$O_2 \rightarrow 2O$	493.59±0.4	117.97±0.1	
$O_3 \rightarrow O_2 + O$	101.4±2.1	24.24±0.5	
$H_2 \rightarrow 2H$	432.00±0.04	103.25±0.01	
$HO \rightarrow H + O$	423.8±2.1	101.3±0.5	
$HO_2 \rightarrow HO + O$	230±8	67±2	
$\rightarrow H + O_2$	210±8	50±2	
$H_2O \rightarrow HO + H$	493.7±0.8	118.0±0.2	
$H_2O_2 \rightarrow 2HO$	207.1±2.1	49.5±0.5	
$H_2O_2 \rightarrow H + HO_2$	350±8	84±2	
$N_2 \rightarrow N + N$	941.69±0.04	225.07±0.01	
$NO \rightarrow N + O$	627.9	150.1	
$NO_2 \rightarrow NO + O$	300.5	71.83	
$NO_3 \rightarrow NO_2 + O$	205±21	49±5	
$N_2O \rightarrow N + NO$	474.9±4	113.5±1	
$\rightarrow N_2 + O$	161.3	38.58	
$N_2O_3 \rightarrow NO + NO_2$	35.1±0.8	8.4±0.2	
$N_2O_4 \rightarrow NO_2 + NO_2$	53.2	12.7	
$N_2O_5 \rightarrow NO_2 + NO_3$	89.5	21.4	
$HNO \rightarrow H + NO$	203	48.6	
$\rightarrow NH + O$	487	116.5	
$trans-HNO_2 \rightarrow HO + NO$	202	48.4	
$HNO_3 \rightarrow HO + NO_2$	200	47.8	
$NH \rightarrow H + N$	343	82	

Bond Dissociation Energies,  $D_0^0$  at 0 K  
Calculated from heats of formation in the accompanying table

Reaction	kJ/mol	kcal/mol	Note
$\text{NH}_2 \rightarrow \text{H} + \text{HN}$	366	87.4	
$\text{NH}_3 \rightarrow \text{NH}_2 + \text{H}$	448	107	
$\text{CO} \rightarrow \text{C} + \text{O}$	1071.94±0.4	256.2±0.1	
$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	525.9±0.4	125.7±0.1	
$\text{CHO} \rightarrow \text{CO} + \text{H}$	70	16.7	(1)
$\text{CH}_2\text{O} \rightarrow \text{CHO} + \text{H}$	364	87	(1)
$\text{CH}_3\text{O} \rightarrow \text{CH}_3 + \text{O}$	378	90.4	(1)
$\quad \rightarrow \text{H} + \text{H}_2\text{CO}$	93	22	(1)
$\text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + \text{O}$	237	56.8	(1)
$\quad \rightarrow \text{CH}_3 + \text{O}_2$	118	28.1	(1)
$\text{CH}_4 \rightarrow \text{CH}_3 + \text{H}$	432	103.2	
$\text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O} + \text{HO}$	184.	44.0	(1)
$\quad \rightarrow \text{CH}_3 + \text{HO}_2$	276±8	66±2	(1)
$\text{CH}_3\text{ONO} \rightarrow \text{CH}_3 + \text{NO}_2$	248	59.2	(1)
$\text{CH}_3\text{NO}_2 \rightarrow \text{CH}_3 + \text{NO}_2$	254	60.6	(1)
$\text{CH}_3\text{ONO}_2 \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	174	41.6	(1)
$\quad \rightarrow \text{CH}_3 + \text{NO}_3$	341	81.6	(1)
$\text{SO} \rightarrow \text{S} + \text{O}$	515.4±8	123.2±2	
$\text{SO}_2 \rightarrow \text{SO} + \text{O}$	547.3±8	130.8±2.0	
$\text{SO}_3 \rightarrow \text{SO}_2 + \text{O}$	342.7±4	81.9±1	

Note 1. Calculated for T = 298K



APPENDIX 2. CONVERSION TABLES  
EQUIVALENT SECOND ORDER RATE CONSTANTS

A \ B	$\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$	$\text{dm}^3 \text{mol}^{-1} \text{s}^{-1}$	$\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$	$\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	$(\text{mm Hg})^{-1} \text{s}^{-1}$	$\text{atm}^{-1} \text{s}^{-1}$	$\text{ppm}^{-1} \text{min}^{-1}$	$\text{m}^2 \text{KN}^{-1} \text{s}^{-1}$
$1 \text{ cm}^3 \text{mol}^{-1} \text{s}^{-1} =$	1	$10^{-3}$	$10^{-6}$	$1.66 \times 10^{-24}$	$1.604 \times 10^{-5} \text{T}^{-1}$	$1.219 \times 10^{-2} \text{T}^{-1}$	$2.453 \times 10^{-9}$	$1.203 \times 10^{-4} \text{T}^{-1}$
$1 \text{ dm}^3 \text{mol}^{-1} \text{s}^{-1} =$	$10^3$	1	$10^{-3}$	$1.66 \times 10^{-21}$	$1.604 \times 10^{-2} \text{T}^{-1}$	$12.19 \text{T}^{-1}$	$2.453 \times 10^{-6}$	$1.203 \times 10^{-1} \text{T}^{-1}$
$1 \text{ m}^3 \text{mol}^{-1} \text{s}^{-1} =$	$10^6$	$10^3$	1	$1.66 \times 10^{-18}$	$16.04 \text{T}^{-1}$	$1.219 \times 10^4 \text{T}^{-1}$	$2.453 \times 10^{-3}$	$120.3 \text{T}^{-1}$
$1 \text{ cm}^3 \text{molecule}^{-1} \text{s}^{-1} =$	$6.023 \times 10^{23}$	$6.023 \times 10^{20}$	$6.023 \times 10^{17}$	1	$9.658 \times 10^{18} \text{T}^{-1}$	$7.34 \times 10^{21} \text{T}^{-1}$	$1.478 \times 10^{15}$	$7.244 \times 10^{19} \text{T}^{-1}$
$1 (\text{mm Hg})^{-1} \text{s}^{-1} =$	$6.236 \times 10^4 \text{T}$	$62.36 \text{T}$	$6.236 \times 10^{-2} \text{T}$	$1.035 \times 10^{-19} \text{T}$	1	760	$4.56 \times 10^{-2}$	7.500
$1 \text{ atm}^{-1} \text{s}^{-1} =$	82.06 T	$8.206 \times 10^{-2} \text{T}$	$8.206 \times 10^{-5} \text{T}$	$1.362 \times 10^{-22} \text{T}$	$1.316 \times 10^{-3}$	1	$6 \times 10^{-5}$	$9.869 \times 10^{-3}$
$1 \text{ ppm}^{-1} \text{min}^{-1} =$ at 298K, 1 atm. total pressure	$4.077 \times 10^8$	$4.077 \times 10^5$	407.7	$6.76 \times 10^{-16}$	21.93	$1.667 \times 10^4$	1	164.5
$1 \text{ m}^2 \text{KN}^{-1} \text{s}^{-1} =$	8314 T	$8.314 \text{T}$	$8.314 \times 10^{-3} \text{T}$	$1.38 \times 10^{-20} \text{T}$	0.1333	101.325	$6.079 \times 10^{-3}$	1

To convert a rate constant from one set of units A to a new set B find the conversion factor for the row A under Column B and multiply the old value by it, e.g. to convert  $\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$  to  $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$  multiply by  $6.023 \times 10^{17}$ .

Table adapted from Evaluated Kinetic Data for High Temperature Reactions, Volume 1: Homogeneous Gas Phase Reactions of the  $\text{H}_2\text{-O}_2$  System, Butterworths, London, 1972.

# EQUIVALENT THIRD ORDER RATE CONSTANTS

A \ B	$6 \text{ cm mol}^{-2} \text{ s}^{-1}$	$6 \text{ dm mol}^{-2} \text{ s}^{-1}$	$6 \text{ mol}^{-2} \text{ s}^{-1}$	$6 \text{ cm molecule}^{-2} \text{ s}^{-1}$	$(\text{mm Hg})^{-2} \text{ s}^{-1}$	$\text{atm}^{-2} \text{ s}^{-1}$	$\text{ppm}^{-2} \text{ min}^{-1}$	$4 \text{ m KN}^{-2} \text{ s}^{-1}$
$1 \text{ cm mol}^{-2} \text{ s}^{-1} =$	1	$10^{-6}$	$10^{-12}$	$2.76 \times 10^{-48}$	$2.57 \times 10^{-10} \text{ T}^{-2}$	$1.48 \times 10^{-4} \text{ T}^{-2}$	$1.003 \times 10^{-19}$	$1.447 \times 10^{-8} \text{ T}^{-2}$
$1 \text{ dm mol}^{-2} \text{ s}^{-1} =$	$10^6$	1	$10^{-6}$	$2.76 \times 10^{-42}$	$2.57 \times 10^{-4} \text{ T}^{-2}$	$148 \text{ T}^{-2}$	$1.003 \times 10^{-13}$	$1.447 \times 10^{-2} \text{ T}^{-2}$
$1 \text{ m mol}^{-2} \text{ s}^{-1} =$	$10^{12}$	$10^6$	1	$2.76 \times 10^{-36}$	$257 \text{ T}^{-2}$	$1.48 \times 10^8 \text{ T}^{-2}$	$1.003 \times 10^{-7}$	$1.447 \times 10^4 \text{ T}^{-2}$
$1 \text{ cm molecule}^{-2} \text{ s}^{-1} =$	$3.628 \times 10^{47}$	$3.628 \times 10^{41}$	$3.628 \times 10^{35}$	1	$9.328 \times 10^{37} \text{ T}^{-2}$	$5.388 \times 10^{43} \text{ T}^{-2}$	$3.64 \times 10^{28}$	$5.248 \times 10^{39} \text{ T}^{-2}$
$1 (\text{mm Hg})^{-2} \text{ s}^{-1} =$	$3.89 \times 10^{9.2} \text{ T}^{-2}$	$3.89 \times 10^{3.2} \text{ T}^{-2}$	$3.89 \times 10^{-3.2} \text{ T}^{-2}$	$1.07 \times 10^{-38.2} \text{ T}^{-2}$	1	$5.776 \times 10^5$	$3.46 \times 10^{-5}$	56.25
$1 \text{ atm}^{-2} \text{ s}^{-1} =$	$6.733 \times 10^{3.2} \text{ T}^{-2}$	$6.733 \times 10^{-3.2} \text{ T}^{-2}$	$6.733 \times 10^{-9.2} \text{ T}^{-2}$	$1.86 \times 10^{-44.2} \text{ T}^{-2}$	$1.73 \times 10^{-6}$	1	$6 \times 10^{-11}$	$9.74 \times 10^{-5}$
$1 \text{ ppm}^{-2} \text{ min}^{-1} =$ at 298K, 1 atm. total pressure	$9.97 \times 10^{18}$	$9.97 \times 10^{12}$	$9.97 \times 10^6$	$2.75 \times 10^{-29}$	$2.89 \times 10^4$	$1.667 \times 10^{10}$	1	$1.623 \times 10^6$
$1 \text{ m KN}^{-2} \text{ s}^{-1} =$	$6.91 \times 10^{7.2} \text{ T}^{-2}$	$69.1 \text{ T}^{-2}$	$6.91 \times 10^{-5.2} \text{ T}^{-2}$	$1.904 \times 10^{-40.2} \text{ T}^{-2}$	0.0178	$1.027 \times 10^4$	$6.16 \times 10^{-7}$	1

See note to Table for Second Order Rate Constants

CONVERSION FACTORS FOR UNITS OF OPTICAL ABSORPTION COEFFICIENTS

B A	(cross section $\sigma$ ) $\frac{2}{\text{cm molecule}}^{-1}$ base e	(atm at 273) $^{-1}$ cm base e	$\frac{3}{\text{dm mol}}^{-1}$ cm $^{-1}$ base 10	$\frac{2}{\text{cm mol}}^{-1}$ base 10
1 (atm at 298) $^{-1}$ cm $^{-1}$ base e =	$4.06 \times 10^{-20}$	1.09	10.6	$1.06 \times 10^4$
1 (atm at 298) $^{-1}$ cm $^{-1}$ base 10 =	$9.35 \times 10^{-20}$	2.51	24.4	$2.44 \times 10^4$
1 (mm Hg at 298) $^{-1}$ cm $^{-1}$ base 10 =	$7.11 \times 10^{-17}$	$1.91 \times 10^3$	$1.86 \times 10^4$	$1.86 \times 10^7$
1 (atm at 273) $^{-1}$ cm $^{-1}$ base e =	$3.72 \times 10^{-20}$	1	9.73	$9.73 \times 10^3$
1 (atm at 273) $^{-1}$ cm $^{-1}$ base 10 =	$8.57 \times 10^{-20}$	2.303	22.4	$2.24 \times 10^4$
1 dm $^3$ mol $^{-1}$ cm $^{-1}$ base 10 =	$3.82 \times 10^{-21}$	0.103	1	$10^3$
1 cm $^2$ mol $^{-1}$ base 10 =	$3.82 \times 10^{-24}$	$1.03 \times 10^{-4}$	$10^{-3}$	1
1 cm $^2$ molecule $^{-1}$ base e =	1	$2.69 \times 10^{19}$	$2.62 \times 10^{20}$	$2.62 \times 10^{23}$

To convert an absorption coefficient from one set of units A to a new set B, multiply by the value tabulated for row A under column B, e.g. to convert the value of the absorption coefficient expressed in dm $^3$  mol $^{-1}$  cm $^{-1}$  base 10 to (atm at 273) $^{-1}$  cm $^{-1}$  base e, multiply by 0.103.

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